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date: June 10, 1996

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subject: 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

INTRODUCTION

This memorandum contains ranges and probability distributions of matrix distribution coefficients (K_ds) for dissolved Pu, Am, U, Th, and Np under conditions expected during transport in the Culebra Dolomite member of the Rustler Formation. In this memo, 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). Performance-assessment (PA) personnel require K_ds for Pu, Am, U, Th, and Np for their calculations to support the Waste Isolation Pilot Plant (WIPP) Compliance Certification Application (CCA) (Ramsey, 1996). (We will include this memorandum and all of the other memoranda cited herein in the parameter and analysis records packages for these K_ds.) Actually, PA requires K_ds for various isotopes of these elements, but Ramsey (1996) did not specify them. However, Garner (1996) stated that PA needs K_ds 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 submitting K_ds for Np in case PA requires them for sensitivity calculations to show that omitting this element does 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, have established these ranges and distributions from results obtained by the RRP through May 31, 1996 (see Table 1 below). These ranges and distributions pertain to dolomite-rich rock in the matrix (intact rock between the fractures) of the Culebra. (We use the terms

SWCF-A:1.1.1D.3.1: PDD: QA: Culebra Dissolved Actinide Distribution Coefficients (Kds), WPO# 38231

"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.) The ranges and distributions in Table 1 *do not* 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 Sewards (1991) and Sewards 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 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.

MATRIX K_ds

This section briefly describes the laboratory studies used to determine matrix K_ds 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 methodologies used to establish ranges and probability distributions of these K_ds.

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 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 with this memo.) Detailed descriptions of these laboratory studies and the complete results will appear as SNL and/or SNL subcontractor reports by the time of 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, developed by Molecke (1983) to simulate fluids equilibrated with K- and Mg-bearing minerals in overlying potash-rich zones in the Salado Formation prior to entering WIPP disposal rooms, 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$_{CO2}$ calculated for Culebra ground waters 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$_d$s versus the final dissolved radionuclide concentration. (We will include these isotherms in the parameter and analysis records packages for these K$_d$s.) 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 to be 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 to be 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 have 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 ground-water 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 the same 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 ^{3}H or [22]Na) and those of U and Np yielded discrete values for the retardation factors 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 by sorption, 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 for Pu and Am, and 19.1, 21.0, and 34.2 pore volumes for Th). Therefore, he was only able to calculate minimum values of R and K_d. 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.

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 are necessary to establish ranges and probability distributions of matrix K_ds 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 have 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 is 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 will ensure 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 will in turn obviate 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 model for Culebra flow and transport.

ASTP and PA personnel will calculate solubilities for *either* Pu(III), U(IV), and Np(IV), *or* Pu(IV), U(VI), and Np(V) in any given vector. PA will specify 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 is 0.5 or less, PA will use the solubilities predicted for Pu(III), U(IV), and Np(IV). (These solubilities are also sampled parameters.) If oxstat is greater than 0.5, PA will use solubilities for Pu(IV), U(VI), and Np(V). We recommend 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 is 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 is 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 are 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 ground water on the order of hundreds of meters from the point of injection.

We are submitting these ranges and distributions to PA concurrently with the submission of Culebra hydrologic parameters by personnel from Geohydrology Department 6115. Therefore, we could not 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 Ranges of Matrix K_ds

This subsection briefly describes the methods used to establish ranges of matrix K_ds 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 empirical-sorption, mechanistic-sorption, and column-transport data considered and included or excluded, appear in Appendices B through F, respectively. Appendix G contains the results of experiments on the effects of four organic ligands on these K_ds.

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 ground waters 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 , 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 K_ds.) 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 revised 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_ds for these elements. In most cases, the K_ds 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 revised 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_ds 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_ds. 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_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) (Table 1); for this recommendation, we invoke the oxidation-state analogy.

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 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

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 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 ranges for deep and Culebra brines in Table 1 reveals that these ranges span 1.40 and 2.60 orders of magnitude (deep and Culebra brines, respectively) for Pu(III) and Am(III); 1.35 orders of magnitude (deep brines only) for Pu(IV), U(IV), Th(IV), and Np(IV); 3.00 orders of magnitude (deep brines only) for U(VI); and 2.65 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 range for U(VI) and Culebra brines because its minimum value is 0.) Because these 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 Range of Matrix K_ds for Use in PA Calculations

We recommend that PA personnel use the 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 have recommended that PA use a uniform distribution for *all* the ranges (see Methods Used to Establish Probability Distributions of Matrix K_ds above), the *average* K_d that PA will 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 ranges for deep and Culebra brines to determine which range results in less retardation for each element or elemental oxidation state. Inspection of the ranges in Table 1 reveals that the means are 260 and 2005 ml/g (deep and Culebra brines, respectively) for Pu(III) and Am(III); 10,450 ml/g (deep brines only) for Pu(IV), U(IV), Th(IV), and Np(IV); 15.015 and 35 ml/g (deep and Culebra brines, respectively) for U(VI); and 451 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 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 that PA use a range of 20 to 500 ml/g (the range for deep brines) for Pu(III) and Am(III); a range of 900 to 20,000 ml/g (deep brines) for Pu(IV), U(IV), Th(IV), and Np(IV); a range of 0.03 to 30 ml/g (deep brines) for U(VI); and a range of 1 to 200 ml/g (Culebra brines) for Np(V). In Table 1, these ranges appear in bold font.

Because the ASTP has 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 range and distribution for each specified oxidation state will constitute the range and distribution for each of these elements during a given vector.

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Table 1. Ranges of Matrix K_ds (ml/g) for Pu, Am, U, Th, and Np, and Dolomite-Rich Culebra Rcok. 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 memo by D. A. Lucero and G. O. Brown dated April 5, 1996. Table checked by Behl on April 8, 1996.

Oxidation State	Element				
	Pu	Am	U	Th	Np
VI	NA	NA	**0.03 to 30**[A,C] 0 to 70[B,C]	NA	NA
V	NA	NA	NA	NA	**2 to 900;**[A,C] 1 to 200[B,C]
IV	**900 to 20,000;**[A,D] NE	NA	**900 to 20,000;**[A,E] NE	**900 to 20,000;**[A,C] NE	**900 to 20,000;**[A,G] NE
III	**20 to 500;**[A,H] 10 to 4,000[B,H]	**20 to 500;**[A,I] 10 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).
NA: not applicable (element will not speciate in this oxidation state).
NE: not established for Culebra brines (see Appendix E).

APPENDIX A: MEETING TO ESTABLISH RANGES AND PROBABILITY
DISTRIBUTIONS OF ACTINIDE K_ds 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_ds 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_ds 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.

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:

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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_ds by PA	M. S. Tierney, SNL
11:45 - 13:00	Lunch	BDM Cafeteria
13:00 - 15:00	Discussion of Range and Distribution of K_ds for Pu(V)	All participants
15:00 - 15:15	Break	
15:15 - 17:15	Discussion of Range and Distribution of K_ds for Am(III) and Pu(III)	All participants

Agenda (continued)

Tuesday, April 2

Time		
8:00 - 10:00	Discussion of Range and Distribution of K_ds 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_ds 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_ds for U(VI) (continued)	All participants
13:30 - 13:45	Break	
13:45 - 15:45	Discussion of Range and Distribution of K_ds for Np(V)	All participants

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

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_ds for Am(III) (see Methods Used to Establish Ranges of Matrix K_ds 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_ds 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% CO_2) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_ds 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 ^{239}Pu in a standard and that in a control exceeded 3σ, 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 22.7 ml/g (from #6004) to 459 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% CO_2) and in glove boxes with atmospheres containing 0.24 and 1.4% CO_2 (see Methods Used to Establish Ranges of Matrix K_ds). 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 ^{239}Pu in a standard and that in a control exceeded 3σ, to obtain the *initial* range of 9.61 ml/g (from #12007) to 3,620 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_ds). Brady's data for 0.5 M NaCl, atmospheric CO_2, and the highest pH values under these conditions are (to three significant figures) 350 and 411 ml/g at a pH of 9.87 and 9.88, respectively (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 22.7 to 459 ml/g and 9.61 to 3,620 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 and his colleagues submitted their results on March 28, 1996, (see Table B-6), then revised them on April 5 and 16, 1996 (Tables B-7 and B-8, respectively). The minimum K_ds reported for experiments C-3, D3, and E-2 (Table B-8) *are consistent with the K_ds reported by Triay for Pu(V) and AISinR 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 22.7 to 459 ml/g and 9.61 to 3,620 ml/g for the deep and Culebra brines, respectively. However, we rounded these ranges to 20 to 500 ml/g and 10 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_ds above).

Furthermore, we recommend that PA use the range of 20 to 500 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_ds for Use in PA Calculations above).

Finally, we recommend that PA use a range of 20 to 500 ml/g for Pu(III) and Am(III) (see Methods Used to Establish Ranges of Matrix K_ds and Appendix C).

Table B-1. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Pu(V), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. No K_ds 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. Table checked by L. J. Storz on June 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	1.98×10^{-7} to 2.39×10^{-7}	22.7, #6004	23.7, #24004	31.9, #12004	28.3 #18004
Brine A	1.11×10^{-8} to 5.28×10^{-8}	54.9, #6024	261, #24024	38.5, #12024	35.9 #18024
Brine A	2.38×10^{-8} to 3.16×10^{-8}	28.0, #6044	34.6, #24044	43.9 #12044	39.4 #18044
Brine A	3.78×10^{-9} to 7.03×10^{-9}	27.2, #6064	30.5, #24064	65.0 #12064	32.1 #18064
Brine A	3.08×10^{-9} to 3.37×10^{-9}	28.6, #6084	30.5, #24084	31.2 #12084	30.3 #18084

Table B-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_ds for Pu(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. Table checked by L. J. Storz on June 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	1.45×10^{-9} to 6.01×10^{-8}	459, #6005	6,890, #24005	7,070, #12005	151 #18005
ERDA-6	3.88×10^{-10} to 1.24×10^{-8}	**3,920,** **#6025**	**6,500,** **#24025**	6,960 #12025	205 #18025
ERDA-6	2.36×10^{-10} to 6.35×10^{-9}	**2,980,** **#6045**	**3,040,** **#24045**	7,540 #12045	253 #18045
ERDA-6	1.59×10^{-10} to 1.67×10^{-9}	**677,** **#6065**	1,140, #24065	1,970 #12065	170 #18065
ERDA-6	3.29×10^{-11} to 1.20×10^{-10}	147, #6085	**1,180,** **#24085**	**1,460** **#12085**	4,550 #18085

Table B-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_ds for Pu(V), Dolomite-Rich Culebra Rock, and AISinR (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. Table checked by L. J. Storz on June 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	1.76×10^{-9} to 9.71×10^{-8}	**348, #6006**	**62.5, #24006**	1,890, #12006	4,100 #18006
AISinR	4.22×10^{-10} to 3.91×10^{-8}	1,990, #6026	37.2, #24026	1,050 #12026	5,050, #18026
AISinR	1.91×10^{-10} to 1.85×10^{-8}	221, #6046	39.8, #24046	3,620 #12046	6,260 #18046
AISinR	1.20×10^{-10} to 3.18×10^{-9}	435, #6066	**50.3, #24066**	848 #12066	1,910 #18066
AISinR	8.43×10^{-11} to 1.93×10^{-9}	499, #6086	42.9, #24086	1,070, #12086	1,360 #18086

Table B-4. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Pu(V), Dolomite-Rich Culebra Rock, and H-17 (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. Table checked by L. J. Storz on June 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	5.94×10^{-8} to 3.01×10^{-7}	**157,** **#6007**	89.5, #24007	9.61, #12007	26.7 #18007
H-17	4.55×10^{-9} to 7.16×10^{-8}	191, #6027	155, #24027	13.3 #12027	33.5 #18027
H-17	3.80×10^{-9} to 3.18×10^{-8}	332, #6047	183, #24047	**14.3** **#12047**	36.6 #18047
H-17	9.35×10^{-10} to 5.48×10^{-9}	256, #6067	182, #24067	25.2 #12067	43.7 #18067
H-17	2.01×10^{-10} to 2.00×10^{-9}	235, #6087	637, #24087	93.9 #12087	45.8 #18087

Table B-5. Effects of pH and P_{CO2} on Matrix K_ds 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.

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
9.88	410.9	NA	NA
9.87	349.56	NA	NA
8.42	0	NA	NA
6.7	-44.928	NA	NA
6.2	34.662	NA	NA
5.81	34.662	NA	NA
5.21	34.662	NA	NA
4.62	128.72	NA	NA
4.05	-113.15	NA	NA
3.51	-44.928	NA	NA
3.11	-310.23	NA	NA

NA: not applicable.

Table B-5. Effects of pH and P_{CO2} on Matrix K_ds 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	465.69	NA
8.49	NA	3711.1	NA
7.32	NA	1029.4	NA
7.19	NA	1162.5	NA
6.99	NA	968.83	NA
6.88	NA	418.41	NA
6.55	NA	319.12	NA
6.17	NA	570.38	NA
5.28	NA	199.2	NA
3.97	NA	99.265	NA
3.13	NA	99.265	NA

NA: not applicable.

Table B-5. Effects of pH and P_{CO2} on Matrix K_ds 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
6.39	NA	NA	124.82
6.91	NA	NA	499.76
6.89	NA	NA	NR
6.8	NA	NA	499.76
6.75	NA	NA	520.02
6.84	NA	NA	371.73
6.49	NA	NA	423.82
6.07	NA	NA	222.63
5.76	NA	NA	147.77
4.91	NA	NA	22.561
3.62	NA	NA	124.82

NA: not applicable.
NR: not reported.

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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 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}	Poro- sity (%)	$K_{d, min}$ (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 1996. Table checked by Y Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/ min)	Run Time (days)	Effluent 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 on memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 1996. Table checked by Y Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on memo by Brown dated April 16, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/ min)	Run Time (days)	Effluent 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.

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_ds 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% CO_2) 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: #6012, #6032, #6052, #6072, and #6092 (see Table C-1), and #6013, #6033, #6053, #6073, and #6093 (see Table C-2 below). We discarded the data from #6012, #6032, #6013, #6033, #6073, and #6093, the runs in which the difference between the activity of the ^{243}Am in a standard and that in a control exceeded 3σ, where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_ds.) Even after discarding the results of these six runs, however, the defensibility of the remaining data is questionable because the K_ds retained for Brine A increase significantly as the final dissolved concentration of ^{243}Am increases. (We will include these isotherms in the parameter and analysis records packages for these K_ds. 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_ds are also proportional to the final dissolved ^{243}Am concentration in the runs carried out in the glove box with an atmosphere containing 1.4% CO_2, and, based on the trends observed with *both* retained and discarded data, *appeared* to increase similarly in the runs conducted in the glove boxes with atmospheres containing 0.24 and 4.1% CO_2 (see Table C-1). Moreover, based on the trends observed with *both* retained and discarded data, these K_ds also *appear* proportional to the final dissolved ^{243}Am concentration at all four CO_2 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 μm, 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 3σ 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% CO_2 to determine, if possible, what caused these trends, and to redetermine these K_ds. 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's 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), were all "high" above a pH of about 5 or 6. ("High" means that insufficient ^{243}Am remained in solution after these runs to determine a K_d). Moreover, although Brady *did* obtain 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.

REFERENCE

Canepa, J.A.   1992.   *Proceedings of the DOE/Yucca Mountain Site Characterization Project Radionuclide Adsorption Workshop at Los Alamos National Laboratory, September 11-12, 1990.*   LA-12325-C.   Los Alamos, NM: Los Alamos National Laboratory.

Table C-1. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Am(III), 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 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. Table checked by L. J. Storz on June 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	1.72×10^{-9} to 2.95×10^{-9}	**965, #6012**	**1,040, #24012**	1,320, #12012	**1,260, #18012**
Brine A	1.13×10^{-9} to 1.47×10^{-9}	**927, #6032**	**1,120, #24032**	1,140, #12032	**1,070, #18032**
Brine A	4.64×10^{-10} to 5.61×10^{-10}	509, #6052	521, #24052	553, #12052	597, #18052
Brine A	3.31×10^{-10} to 4.14×10^{-10}	330, #6072	356, #24072	392, #12072	346, #18072
Brine A	2.65×10^{-10} to 3.24×10^{-10}	67.9, #6092	**76.6, #24092**	86.8, #12092	77.8, #18092

Table C-2. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Am(III), 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. Table checked by L. J. Storz on June 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	2.18×10^{-10} to 4.66×10^{-10}	**5,620,** **#6013**	**9,590,** **#24013**	10,800, #12013	**5,230,** **#18013**
ERDA-6	1.57×10^{-10} to 7.10×10^{-10}	**5,100,** **#6033**	**4,760,** **#24033**	**8,110,** **#12033**	**2,080,** **#18033**
ERDA-6	1.06×10^{-10} to 2.02×10^{-10}	1,650, #6053	1,610, #24053	**2,010,** **#12053**	**1,210,** **#18053**
ERDA-6	1.22×10^{-10} to 1.51×10^{-10}	**978,** **#6073**	**877,** **#24073**	832, #12073	**754,** **#18073**
ERDA-6	9.23×10^{-11} to 1.16×10^{-10}	**211,** **#6093**	272, #24093	**249,** **#12093**	**258,** **#18093**

Table C-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_ds for Am(III), Dolomite-Rich Culebra Rock, and ASIinR (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. Table checked by L. J. Storz on June 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
AISinR	1.14×10^{-9} to 4.02×10^{-9}	**1,790,** **#6014**	730, #24014	**637,** **#12014**	507, #18014
AISinR	6.95×10^{-10} to 2.29×10^{-9}	**1,660,** **#6034**	**594,** **#24034**	676, #12034	504, #18034
AISinR	1.92×10^{-10} to 4.47×10^{-10}	934, #6054	760, #24054	**437,** **#12054**	**436,** **#18054**
AISinR	1.27×10^{-10} to 2.89×10^{-10}	**653,** **#6074**	640, #24074	344, #12074	**334,** **#18074**
AISinR	1.26×10^{-10} to 1.64×10^{-10}	190, #6094	145, #24094	133, #12094	156, #18094

Table C-4. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Am(III), Dolomite-Rich Culebra Rock, and H-17 (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. Table checked by L. J. Storz on June 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	6.35×10^{-10} to 1.69×10^{-9}	**1,590, #6015**	**1,310, #24015**	**688, #12015**	**547, #18015**
H-17	4.42×10^{-10} to 1.77×10^{-9}	**1,140, #6035**	**1,120, #24035**	**622, #12035**	**484, #18035**
H-17	2.27×10^{-10} to 3.60×10^{-10}	**870, #6055**	836, #24055	499, #12055	**633, #18055**
H-17	1.57×10^{-10} to 3.16×10^{-10}	**826, #6075**	626, #24075	418, #12075	**383, #18075**
H-17	1.43×10^{-10} to 3.36×10^{-10}	76.1, #6095	187, #24095	189, #12095	**155, #18095**

Table C-5. Effects of pH and P_{CO2} on Matrix K_ds 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	2864.3	NA	NA
8.41	1619.2	NA	NA
7.52	1225.2	NA	NA
6.72	1141.4	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

NA: not applicable.

Table C-5. Effects of pH and P_{CO2} on Matrix K_ds 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

NA: not applicable.

Table C-5. Effects of pH and P_{CO2} on Matrix K_ds 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_{CO2} on Matrix K_ds 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.

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
9.88	High	NA	NA
9.87	High	NA	NA
8.42	High	NA	NA
6.7	High	NA	NA
6.2	High	NA	NA
5.81	High	NA	NA
5.21	High	NA	NA
4.62	791.15	NA	NA
4.05	630.75	NA	NA
3.51	285.41	NA	NA
3.11	92.603	NA	NA

NA: not applicable.

Table C-6. Effects of pH and P_{CO2} on Matrix K_ds 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	High	NA
8.49	NA	High	NA
7.32	NA	High	NA
7.19	NA	High	NA
6.99	NA	High	NA
6.88	NA	High	NA
6.55	NA	High	NA
6.17	NA	High	NA
5.28	NA	1130.9	NA
3.97	NA	65.441	NA
3.13	NA	158.09	NA

NA: not applicable.

Table C-6. Effects of pH and P_{CO2} on Matrix K_ds 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
6.39	NA	NA	High
6.91	NA	NA	High
6.89	NA	NA	High
6.8	NA	NA	High
6.75	NA	NA	High
6.84	NA	NA	High
6.49	NA	NA	High
6.07	NA	NA	High
5.76	NA	NA	1934.3
4.91	NA	NA	333.78
3.62	NA	NA	-10.908

NA: not applicable.

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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/ min)	Run Time (days)	Effluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 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}	Poro- sity (%)	$K_{d, min}$ (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 1996. Table checked by Y. Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on memo by Brown dated April 16, 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_ds 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_ds 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% CO_2) 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: #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 [233]U in a standard and that in a control exceeded 3σ, where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_ds). Discarding the data from these five runs yielded an *initial* range of 3.76 ml/g (from #6029) to 21.8 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% CO_2) and in glove boxes with atmospheres containing 0.24 and 1.4% CO_2 (see Methods Used to Establish Ranges of Matrix K_ds). 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 [233]U in a standard and that in a control exceeded 3σ, to obtain the *initial* range of -1.66 ml/g (from #12091) to 68.7 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_ds). Brady's data for 0.5 M NaCl, atmospheric CO_2, and the highest

pH values under these conditions are (to three significant figures) 10.6 and 34.7 ml/g at a pH of 9.87 and 9.88, respectively (Table D-5).. Because these values are *greater than the upper 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 3.76 ml/g to 34.7 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 68.7 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 CO_2 content of these experiments was probably similar to that in the LANL bench-top (0.033% CO_2) runs. Lucero *did* observe breakthrough of U(VI) in his experiments. Therefore, it was possible to determine actual K_ds for this element. Lucero and his colleagues submitted their results on March 28, 1996, (see Table D-6), 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 ml/g to 34.7 ml/g, and rounded it to 0.03 to 30 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 68.7 ml/g, rounded to 0 to 70 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 30 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).

Table D-1.—Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for U(VI), 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 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. Table checked by L. J. Storz on June 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	1.65×10^{-6} to 2.81×10^{-6}	**12.5,** **#6008**	**4.77,** **#24008**	**1.16,** **#12008**	0.709, #18008
Brine A	7.89×10^{-7} to 1.05×10^{-6}	**16.8,** **#6028**	2.86, #24028	1.21, #12028	2.67, #18028
Brine A	1.85×10^{-7} to 2.72×10^{-7}	**19.9,** **#6048**	5.23, #24048	1.47, #12048	2.46, #18048
Brine A	7.60×10^{-8} to 1.09×10^{-7}	**16.6,** **#6068**	6.81, #24068	0.933, #12068	2.30, #18068
Brine A	2.14×10^{-8} to 4.16×10^{-8}	21.8, #6088	4.70, #24088	-5.41, #12088	1.44, #18088

Table D-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_ds for U(VI), 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. Table checked by L. J. Storz on June 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	2.62×10^{-6} to 2.99×10^{-6}	**0.542,** **#6009**	1.29, #24009	**4.13,** **#12009**	3.75, #18009
ERDA-6	8.61×10^{-7} to 9.87×10^{-7}	3.76, #6029	1.52, #24029	5.92, #12029	**3.17,** **#18029**
ERDA-6	2.14×10^{-7} to 2.56×10^{-7}	3.86, #6049	2.38, #24049	7.25, #12049	3.22, #18049
ERDA-6	8.40×10^{-8} to 9.28×10^{-8}	3.88, #6069	4.35, #24069	6.24, #12069	4.76, #18069
ERDA-6	2.31×10^{-8} to 2.87×10^{-8}	6.55, #6089	2.11, #24089	7.04, #12089	1.04, #18089

Table D-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_ds for U(VI), Dolomite-Rich Culebra Rock, and ASIinR (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. Table checked by L. J. Storz on June 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	2.86×10^{-6} to 3.04×10^{-6}	**2.56, #6010**	**0.351, #24010**	**0.550, #12010**	**1.67, #18010**
AISinR	9.57×10^{-7} to 1.06×10^{-6}	2.62, #6030	**2.69, #24030**	2.05, #12030	**0.756, #18030**
AISinR	2.63×10^{-7} to 2.87×10^{-7}	**3.74, #6050**	0.389, #24050	1.65, #12050	**3.73, #18050**
AISinR	8.22×10^{-8} to 9.50×10^{-8}	**4.02, #6070**	3.16, #24070	1.03, #12070	**0.341, #18070**
AISinR	2.60×10^{-8} to 2.79×10^{-8}	7.51, #6090	0.117, #24090	1.73, #12090	1.88, #18090

Table D-4. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for U(VI), Dolomite-Rich Culebra Rock, and H-17 (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. Table checked by L. J. Storz on June 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	2.76×10^{-6} to 2.97×10^{-6}	**3.63,** **#6011**	0.313, #24011	**-0.745,** **#12011**	-0.104, #18011
H-17	1.11×10^{-6} to 1.16×10^{-6}	**5.55,** **#6031**	1.30, #24031	0.157, #12031	0.530, #18031
H-17	2.72×10^{-7} to 2.92×10^{-7}	**6.97,** **#6051**	3.03, #24051	**-1.83,** **#12051**	2.26, #18051
H-17	8.73×10^{-8} to 9.86×10^{-8}	**5.12,** **#6071**	1.90, #24071	1.50, #12071	-1.22, #18071
H-17	6.89×10^{-9} to 2.83×10^{-8}	10.2, #6091	68.7, #24091	-1.66, #12091	2.96, #18091

Table D-5. Effects of pH and P_{CO2} on Matrix K_ds 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.

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
9.88	34.662	NA	NA
9.87	10.6	NA	NA
8.42	7691.2	NA	NA
6.7	4794.1	NA	NA
6.2	3345.6	NA	NA
5.81	5685.5	NA	NA
5.21	2476.5	NA	NA
4.62	2476.5	NA	NA
4.05	2621.3	NA	NA
3.51	2342.8	NA	NA
3.11	1897.1	NA	NA

NA: not applicable.

Table D-5. Effects of pH and P_{CO2} on Matrix K_ds 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	775.74	NA
8.49	NA	-112.13	NA
7.32	NA	44.55	NA
7.19	NA	123.88	NA
6.99	NA	286.76	NA
6.88	NA	849.72	NA
6.55	NA	1114	NA
6.17	NA	455.52	NA
5.28	NA	1774.6	NA
3.97	NA	1611.4	NA
3.13	NA	4222.7	NA

NA: not applicable.

Table D-5. Effects of pH and P_{CO2} on Matrix K_ds 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
6.39	NA	NA	475.59
6.91	NA	NA	69.799
6.89	NA	NA	0
6.8	NA	NA	0
6.75	NA	NA	69.799
6.84	NA	NA	69.799
6.49	NA	NA	296.73
6.07	NA	NA	1517.2
5.76	NA	NA	2056.6
4.91	NA	NA	3075.4
3.62	NA	NA	1674.5

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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 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	Poro- sity (%)	K_d (ml/g)	Range ($\pm$ml/ g)
B-3	VPX- 26- 11A	AIS.	0.1	NA	NA	$3.4;^S$ 1, $18.3;^N$ 3.1, 5.2^{DF}	9.8^S 5.2^{DN} 5.2^{DF}	$.084^S$ $\mathbf{0.68^{DN}}$ $.039^{DF}$	$.022^S$ $.67^{DN}$ 0.03^{DF}
B-6	VPX- 26- 11A	AIS.	0.05	NA	NA	$13.1;^S$ 1, $NA;^{DN}$ NA, NA^{DF}	4.8^S NA^{DN} NA^{DF}	0.25^S $\mathbf{NA^{DN}}$ NA^{DF}	0.07^S $\mathbf{NA^{DN}}$ NA^{DF}
C-2	VPX- 28-6C	AIS.	0.1	21	2	$10.4;^S$ 1, $260;^{DN}$ 12.0, 0.6^{DF}	5.7^S 3.5^{DN} 3.5^{DF}	0.23^S $\mathbf{3.9^{DN}}$ 0.17^{DF}	0.08^S 7^{DN} 0.06^{DF}
C-7	VPX- 28-6C	ER.-6	0.1	13	2	$2.7;^S$ 1, $0.6;^{DN}$ 2.7, 0.76^{DF}	3.9^S 2.1^{DN} 2.1^{DF}	$.029^S$ $\mathbf{.069^{DN}}$ $.016^{DF}$	$.022^S$ $\mathbf{0.13^{DN}}$ $.005^{DF}$

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	Poro-sity (%)	K_d (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 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	Poro- sity (%)	K_d (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996 based on memo by Lucero and Brown dated April 5, 1996. Table checked by Y. Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on memo by Brown dated April 16, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Effluent Vol. (L)	R	Porosity (%)	K_d (ml/g)	Range (±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_ds 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_ds 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% CO_2) 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: #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 ^{230}Th in a standard and that in a control exceeded 3σ, where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_ds). Discarding the data from these two runs yielded an *initial* range of 864 ml/g (from #7010A) to 15,000 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% CO_2) and in glove boxes with atmospheres containing 0.24 and 1.4% CO_2 (see Methods Used to Establish Ranges of Matrix K_ds). 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 ^{230}Th in a standard and that in a control exceeded 3σ. Therefore, we assumed that the *initial* range of 864 to 15,000 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 864 to 15,000 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 CO_2 content of these

experiments was probably similar to that in the LANL bench-top (0.033% CO_2) 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_ds 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 ^{228}Th in the effluent is much higher than those for ^{241}Pu and ^{241}Am because of the low yield of the ^{228}Th γ emission; (2) although ^{228}Th 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 ^{228}Th by observing the decay of its daughters, such as ^{224}Ra, was not possible because of interference by identical daughters produced by the decay of ^{232}U, which was used in all of the cores. Lucero and his colleagues submitted their results on March 28, 1996, (Table E-5), then revised them on April 5, 1996 (Table E-6). The minimum K_ds 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 864 to 15,000 ml/g, rounded to 900 to 20,000 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_ds above).

Finally, based on the oxidation-state analogy, we recommend that PA use a range of 900 to 20,000 ml/g for Pu(IV), U(IV), and Np(IV) (see Table 1).

Table E-1. Effects of Initial Radionuclide Concentration and P_{CO2} 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.

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	**313, #7011A**	**205, #7053A**	**338, #7025A**	**694, #7039A**
Brine A	NA	**250, #7011B**	**227, #7053B**	**352, #7025B**	**706, #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_ds for Th(IV), 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 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.

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	5,340, #7007A	**6,600, #7049A**	12,900, #7021A	4,600, #7035A
ERDA-6	NA	5,270, #7007B	**8,950, #7049B**	15,900, #7021B	7,060, #7035B
ERDA-6	NA	6,650, #7008A	**8,720, #7050A**	8,670, #7022A	**7,340, #7036A**
ERDA-6	NA	15,000, #7008B	**6,450, #7050B**	7,780, #7022B	**9,620, #7036B**
ERDA-6	NA	2,180, #7009A	1,640, #7051A	14,100, #7023A	6,810, #7037A
ERDA-6	NA	2,820, #7009B	3,740, #7051B	7,270, #7023B	45,600, #7037B
ERDA-6	NA	864, #7010A	1,930, #7052A	High, #7024A	364, #7038A
ERDA-6	NA	1,300, #7010B	1,780, #7052B	1,130, #7024B	2,850, #7038B

NA: not available yet.
ND: not determined.

Table E-3. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Th(IV), Dolomite-Rich Culebra Rock, and AISinR (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.

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**	**10,800, #7054A**	**4,580, #7026A**	**57,100, #7040A**
AISinR	NA	**High, #7012B**	**16,900, #7054B**	**7,080, #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_ds for Th(IV), Dolomite-Rich Culebra Rock, and H-17 (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.

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	**12,100, #7013A**	**7,580, #7055A**	**High, #7027A**	**14,500, #7041A**
H-17	NA	**High, #7013B**	**High, #7055B**	**23,700, #7027B**	**14,300, #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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/ min)	Run Time (days)	Effluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (±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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 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}	Poro- sity (%)	$K_{d, min}$ (ml/g)	Range (±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% CO_2) 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 [237]Np in a standard and that in a control exceeded 3σ, 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 8.64 ml/g (from #6020) to 47.7 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% CO_2) and in glove boxes with atmospheres containing 0.24 and 1.4% CO_2 (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 [237]Np in a standard and that in a control exceeded 3σ, to obtain the *initial* range of 2.09 ml/g (from #12022) to 163 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 CO_2, and the highest pH values under these conditions are (to three significant figures) 892 and 938 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 8.64 to 938 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 2.09 to 163 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 CO_2 content of these experiments was probably similar to that in the LANL bench-top (0.033% CO_2) runs. Lucero *did* observe breakthrough of Np(V) in his experiments. Therefore, it was possible to determine actual K_ds for this element. Lucero and his colleagues submitted their results on March 28, 1996, (see Table F-6), 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 938 ml/g, and rounded it to 2 to 900 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 163 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).

Table F-1. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Np(V), 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 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. Table checked by L. J. Storz on June 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	6.80×10^{-7} to 9.26×10^{-6}	8.64, #6020	5.05, #24020	224, #12020	380, #18020
Brine A	3.86×10^{-6} to 4.52×10^{-6}	**16.1, #6040**	**31.9, #24040**	11.8, #12040	8.91, #18040
Brine A	6.09×10^{-7} to 6.56×10^{-7}	20.3, #6060	**150, #24060**	21.3, #12060	21.9, #18060
Brine A	2.16×10^{-7} to 2.58×10^{-7}	37.5, #6080	32.5, #24080	36.7, #12080	27.0, 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. Table checked by L. J. Storz on June 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	4.43×10^{-7} to 9.85×10^{-7}	**218, #6021**	**241, #24021**	562, #12021	**508, #18021**
ERDA-6	4.81×10^{-7} to 1.46×10^{-6}	**55.2, #6041**	**181, #24041**	153, #12041	**117, #18041**
ERDA-6	1.70×10^{-7} to 5.58×10^{-7}	47.7, #6061	**280, #24061**	163, #12061	29.9, #18061
ERDA-6	8.59×10^{-9} to 2.78×10^{-7}	31.7, #6081	**14,000, #24081**	**High! #12081**	**High! #18081**

ND: not determined.

Table F-3. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Np(V), Dolomite-Rich Culebra Rock, and AISinR (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. Table checked by L. J. Storz on June 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	7.62×10^{-6} to 8.72×10^{-6}	5.12, #6022	3.70, #24022	2.09, #12022	2.19, #18022
AISinR	6.06×10^{-7} to 4.53×10^{-6}	163, #6042	**11.9, #24042**	2.35, #12042	2.23, #18042
AISinR	5.26×10^{-7} to 8.08×10^{-7}	20.4, #6062	9.64, #24062	4.06, #12062	4.83, #18062
AISinR	2.39×10^{-7} to 3.81×10^{-7}	32.9, #6082	**46.7, #24082**	9.89, #12082	10.4, #18082

ND: not determined.

Table F-4. Effects of Initial Radionuclide Concentration and P_{CO2} on Matrix K_ds for Np(V), Dolomite-Rich Culebra Rock, and H-17 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. No K_ds 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. Table checked by L. J. Storz on June 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	2.88×10^{-7} to 9.88×10^{-6}	52.4, #6023	19.0, #24023	2.96, #12023	1.40, #18023
H-17	3.30×10^{-6} to 4.93×10^{-6}	15.8, #6043	13.3, #24043	3.23, #12043	2.37, #18043
H-17	3.44×10^{-7} to 8.87×10^{-7}	40.1, #6063	25.8, #24063	47.1, #12063	4.61, #18063
H-17	2.16×10^{-7} to 8.19×10^{-6}	44.2, #6083	8.02, #24083	3.79, #12083	6.60, #18083

ND: not determined.

Table F-5. Effects of pH and P_{CO_2} on Matrix K_ds 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.

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
9.88	938.1	NA	NA
9.87	891.95	NA	NA
8.42	324.37	NA	NA
6.7	59.493	NA	NA
6.2	59.493	NA	NA
5.81	-6.7249	NA	NA
5.21	59.493	NA	NA
4.62	59.493	NA	NA
4.05	59.493	NA	NA
3.51	59.493	NA	NA
3.11	-6.7249	NA	NA

NA: not applicable.

Table F-5. Effects of pH and P_{CO2} on Matrix K_ds 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	82.353	NA
8.49	NA	623.53	NA
7.32	NA	352.94	NA
7.19	NA	248.87	NA
6.99	NA	248.87	NA
6.88	NA	159.66	NA
6.55	NA	82.353	NA
6.17	NA	159.66	NA
5.28	NA	82.353	NA
3.97	NA	82.353	NA
3.13	NA	159.66	NA

NA: not applicable.

Table F-5. Effects of pH and P_{CO2} on Matrix K_ds 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
6.39	NA	NA	-56.83
6.91	NA	NA	100.36
6.89	NA	NA	0
6.8	NA	NA	100.36
6.75	NA	NA	100.36
6.84	NA	NA	100.36
6.49	NA	NA	100.36
6.07	NA	NA	15.721
5.76	NA	NA	15.721
4.91	NA	NA	100.36
3.62	NA	NA	15.721

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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 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	Poro- sity	K_d (ml/g)	Range (±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]**
						7.0, 103[DF]	2.3[DF]	0.06[DF]	0.03[DF]
C-6	VPX- 28-6C	AIS.	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]**
						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]**
						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]**
						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	Poro- sity	K_d (ml/g)	Range (±ml/ g)
D-4	VPX- 25-8A	AIS.	0.1	13	2	39;[S]	10.0[S]	1.65[S]	0.22[S]
						1, 340;[DN]	4.8[DN]	7.1[DN]	4.2[DN]
						17.5, 154[DF]	4.8[DF]	0.34[DF]	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 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 memo by D. A. Lucero, G. O. Brown, and K. G. Budge dated March 28, 1996. Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on memo by Lucero and Brown dated April 5, 1996. Table checked by Y. Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (mL/ min)	Run Time (days)	Effluent Vol. (L)	R	Porosity	K_d (mL/g)	Range (±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_ds
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_ds 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_ds 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%) CO_2; Am(III), ERDA-6, and 0.033% CO_2; and U(VI), ERDA-6, and 0.033% CO_2, low concentrations of these organic ligands actually *increase* the K_ds relative to those obtained without any organic ligands. However, at high concentrations, these organic ligands significantly *decrease* the K_ds 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_ds 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_ds for Th relative to those obtained without any organics, but had much less effect on the K_ds for the other elements. Intermediate concentrations of organics significantly decreased the K_ds for all of the elements except U(VI). High concentrations significantly decreased the K_ds for all five of these elements.

However, we *have not* revised the ranges and probability distributions of K_ds 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_ds 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 $Mg(OH)_2$, 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. (ERDA-6 and H-17) (mM)	High Conc. (ERDA-6 and H-17) (mM)	Low Conc. (Modified Brine A) (mM)	Intermediate Conc. (Modified Brine A) (mM)	High Conc. (Modified Brine A) (mM)	Predicted Conc. in WIPP (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_{CO2} on Matrix K_ds for Pu(V) and Dolomite-Rich Culebra Rock (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. 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.

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	217, #JRF O-181
ERDA-6	None	158, #JRF O-132	223, #JRF O-182
ERDA-6	Avg. without organics	158	220
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_ds 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	8.51, #JRF O-81
H-17	None	19.8, #JRF O-32	9.19, #JRF O-82
H-17	Avg. without organics	19.1	8.85
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	6.14
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_ds for Am(III) and Dolomite-Rich Culebra Rock (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. 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.

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	2,890, #JRF O-191
ERDA-6	None	1,220, #JRF O-142	2,160, #JRF O-192
ERDA-6	Avg. without organics	710	2,520
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_ds 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_{CO2} on Matrix K_ds for U(VI) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H19, B-4, Box 7. K_ds 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_ds 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.

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	-0.296, #JRF O-159
ERDA-6	None	0.220, #JRF O-112	0.275, #JRF O-160
ERDA-6	Avg. without organics	0.110	0.138
ERDA-6	Low-conc. organics	1.83, #JRF O-119	-0.0367, #JRF O-168
ERDA-6	Low-conc. organics	-0.371, #JRF O-120	-0.933, #JRF O-169
ERDA-6	Avg. w. low-conc. org.	0.915	0.00
ERDA-6	High-conc. organics	-0.631, #JRF O-117	-0.475 #JRF O-166
ERDA-6	High-conc. organics	-0.638, #JRF O-118	-0.948, #JRF O-167
ERDA-6	Avg. w. high-conc. org.	0.000	0.00

Table G-4. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_ds 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_ds for Th(IV) and Dolomite-Rich Culebra Rock (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. 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.

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	153, #JRF O-148
ERDA-6	None	98.6, #JRF O-102	169, #JRF O-149
ERDA-6	Avg. without organics	109	161
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_{CO2} on Matrix K_ds 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	12.0, #JRF O-51
H-17	None	16.6, #JRF O-2	11.3, #JRF O-52
H-17	Avg. without organics	15.8	11.6
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_{CO2} on Matrix K_ds for Np(V) and Dolomite-Rich Culebra Rock (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. 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.

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	136, #JRF O-170
ERDA-6	None	87.6, #JRF O-122	148, #JRF O-172
ERDA-6	Avg. without organics	92.0	142
ERDA-6	Low-conc. organics	83.6, #JRF O-129	175, #JRF O-179
ERDA-6	Low-conc. organics	79.1, #JRF O-130	147, #JRF O-180
ERDA-6	Avg. w. low-conc. org.	81.4	161
ERDA-6	High-conc. organics	63.9, #JRF O-127	131, #JRF O-177
ERDA-6	High-conc. organics	63.3, #JRF O-128	113, #JRF O-178
ERDA-6	Avg. w. high-conc. org.	63.6	122

Table G-6. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_ds 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	0.905, #JRF O-71
H-17	None	4.37, #JRF O-22	1.06, #JRF O-72
H-17	Avg. without organics	4.77	0.983
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.

	Element and Oxidation State				
Additive	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