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**LESSONS LEARNED FROM CHARACTERIZATION, PERFORMANCE
ASSESSMENT, AND EPA REGULATORY REVIEW OF THE 1996 ACTINIDE
SOURCE TERM FOR THE WASTE ISOLATION PILOT PLANT**

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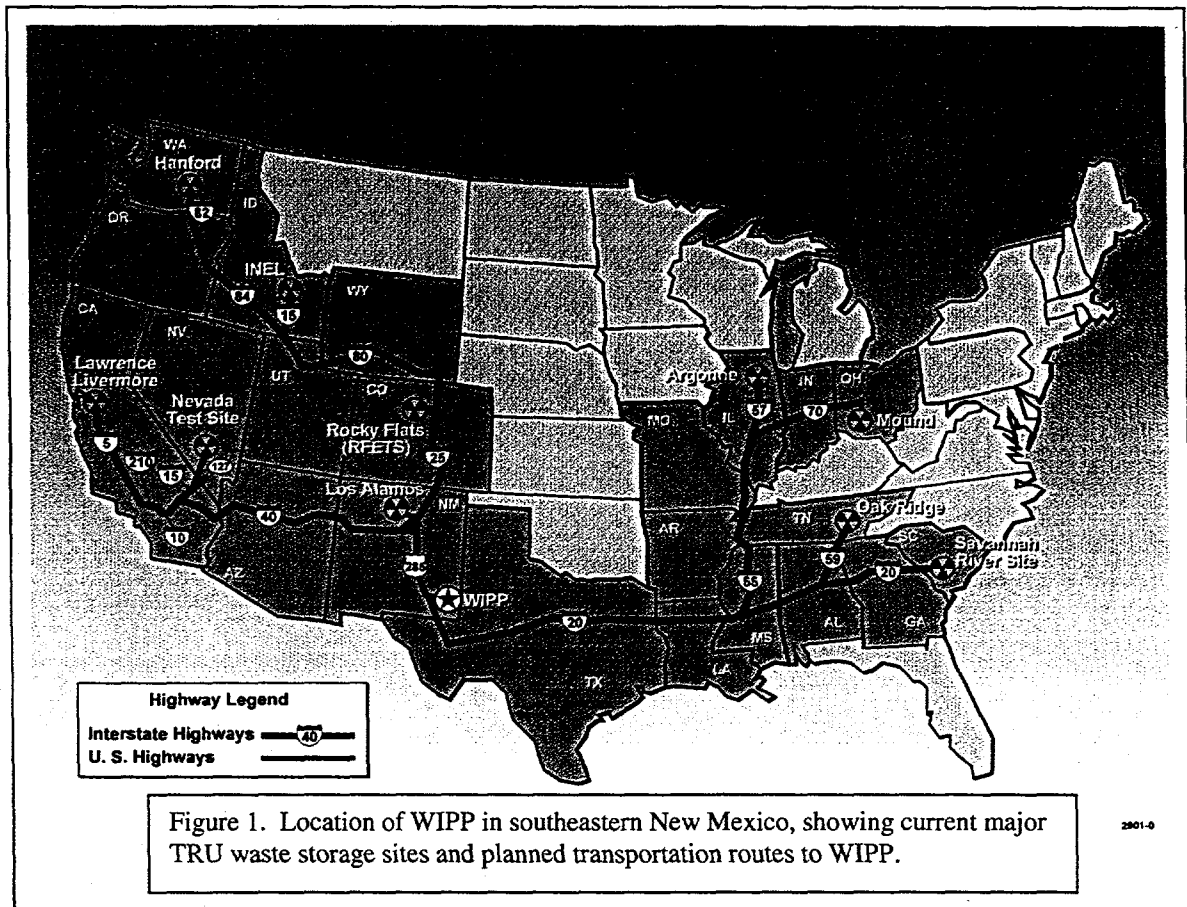
Abstract

The Waste Isolation Pilot Plant (WIPP) is a U.S. Department of Energy (DOE) facility for the permanent disposal of transuranic waste from defense activities. In 1996, the DOE submitted the *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant (CCA)* to the U.S. Environmental Protection Agency (EPA). The CCA included a probabilistic performance assessment (PA) conducted by Sandia National Laboratories to establish compliance with the quantitative release limits defined in 40 CFR 191.13. An experimental program to collect data relevant to the actinide source term began around 1989, which eventually supported the 1996 CCA PA actinide source term model. The actinide source term provided an estimate of mobile dissolved and colloidal Pu, Am, U, Th, and Np concentrations in their stable oxidation states, and accounted for effects of uncertainty in the chemistry of brines in waste disposal areas. The experimental program and the actinide source term included in the CCA PA underwent EPA review lasting more than 1 year. Experiments were initially conducted to develop data relevant to the wide range of potential future conditions in waste disposal areas. Interim, preliminary performance assessments and actinide source term models provided insight allowing refinement of experiments and models. Expert peer review provided additional feedback and confidence in the evolving experimental program. By 1995, the chemical data base and PA predictions of WIPP performance were considered reliable enough to support the decision to add an MgO backfill to waste rooms to control chemical conditions and reduce uncertainty in actinide concentrations, especially for Pu and Am. Important lessons learned through the characterization, PA modeling, and regulatory review of the actinide source term are (1) experimental characterization and PA should evolve together, with neither activity completely dominating the other, (2) the understanding of physical processes required to develop conceptual models is greater than can be represented in PA models, (3) experimentalists should be directly involved in model and parameter abstraction and simplification for PA, and (4) external expert review should be incorporated early in a project to increase confidence long before regulatory reviews begin.

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Introduction

The WIPP is located in semi-arid desert in southeastern New Mexico (Figure 1). It is located in the Salado Formation, a bedded salt, about 650 meters below ground surface (Figure 2). The repository is designed to dispose of approximately 175,000 cubic meters of transuranic waste (materials containing more than 100 nanocuries [3700 becquerels] per gram of transuranic isotopes with half lives greater than 20 years) derived from defense-related activities of the United States government. Total initial activity of the waste (as of 1995) is estimated to be 7.4×10^6 curies (2.7×10^{17} becquerels), with the largest component of this activity coming from isotopes of plutonium.



Evaluations of the suitability of the site for disposal of radioactive waste began in 1974, and extensive site characterization activities were conducted throughout the late 1970s and the 1980s. Although excavation of the underground facilities began in 1981, the process of regulatory certification did not begin until 1992, when the United States Congress established the EPA as the regulator for the WIPP. Following a series of iterative performance assessments in the early 1990s and the subsequent refocusing of scientific programs to support specific compliance-related needs, the DOE submitted a Compliance Certification Application (CCA) to the EPA in October 1996 [1]. The EPA issued a draft certification ruling for public comment in October 1997, and issued the final certification in May 1998. Disposal operations for non-hazardous TRU waste are currently scheduled to begin in 1999, pending resolution of legal issues. Disposal operations for hazardous TRU waste (i.e., waste that is also contaminated with hazardous non-radioactive materials such as volatile organic compounds and heavy metals) are currently scheduled to begin in late 1999, pending receipt of an operating permit from the State of New Mexico.

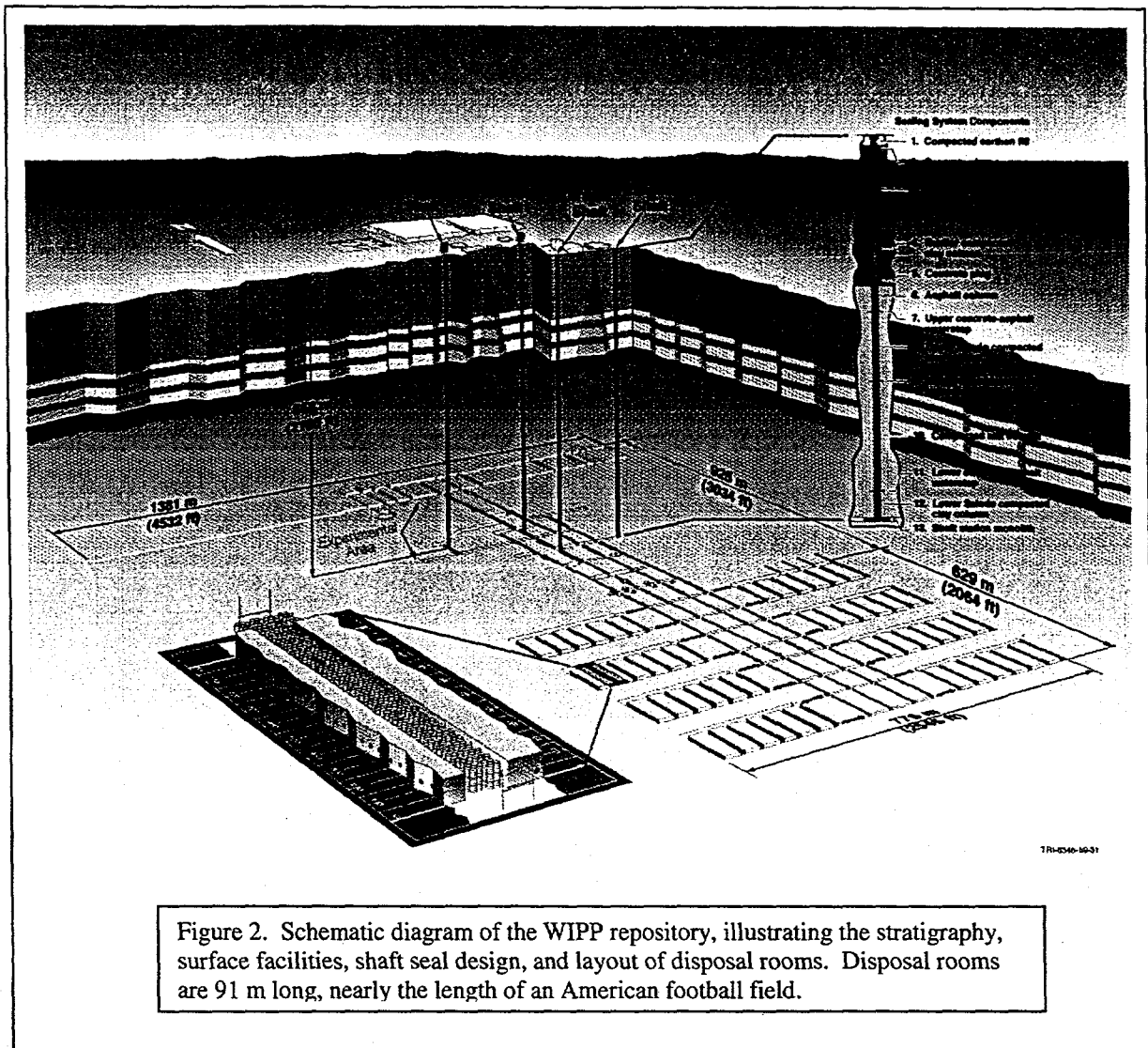


Figure 2. Schematic diagram of the WIPP repository, illustrating the stratigraphy, surface facilities, shaft seal design, and layout of disposal rooms. Disposal rooms are 91 m long, nearly the length of an American football field.

Overview of Chemical Conditions and Actinide Source Term at WIPP¹

The Salado Formation consists predominantly of halite, $\text{NaCl}(s)$, but also contains accessory evaporite minerals such as anhydrite, CaSO_4 , gypsum, $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$, polyhalite, $\text{K}_2\text{MgCa}_2(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$, and magnesite, MgCO_3 , as well as thin layers of fractured anhydrite marker beds and clay seams [2]. The inter- and intragranular brines associated with the salt at the repository horizon are highly concentrated solutions (about 10 times that of sea water) dominated by the ions Na^+ , Mg^{2+} , K^+ , Cl^- , and SO_4^{2-} but also containing smaller amounts of Ca^{2+} , CO_3^{2-} , and B^{3+} [3]. Because these brines have been in contact with the evaporite salts through geologic time they are saturated with respect to the evaporite minerals. For this reason there is little potential that the brines would be capable of further dissolving evaporite minerals in the Salado Formation. The compositional differences between brine in the Salado Formation from point to point are less than about 20%. The Castile Formation is a bedded anhydrite formation underlying the Salado Formation. For PA, it is assumed that brine in the Castile Formation may enter the repository by flow through inadvertent intrusion boreholes drilled for resource exploration. Brines associated with the Castile Formation are predominantly saturated sodium chloride solutions also containing Ca^{2+} , SO_4^{2-} and small concentrations of other elements. Brines in the Castile Formation are about eight times more concentrated than seawater. The major difference between the Castile and Salado brines is the magnesium

¹ This section summarizes concepts and results in the CCA. For details, the reader is encouraged to consult the CCA and the many references cited therein [1].

concentration, which is about 0.02 m in the Castile brines and about 1.0 m in the Salado brines. Near-surface unsaturated liquids in the vicinity of WIPP could also enter the repository by flow through inadvertent intrusion boreholes. These liquids would chemically resemble Castile brine after dissolving Salado salt.

The chemical composition of the brines is a primary factor affecting the chemical fate of the actinides in both the aqueous and solid phases. The two native, approximately uniform, brine compositions from the Salado and Castile Formations may be chemically altered through contact with the disposal system. The inclusion of MgO as a backfill material has the dual purposes of controlling the hydrogen ion concentration and complexing CO₂(g) that may be generated by microbial decay of cellulosic, plastic, and rubber waste material. The MgO should maintain the pH between about 9 and 10 where the actinides will be less soluble than at lower pH values. The introduction of magnesium into the repository will cause precipitation of the carbonate as a hydrated magnesium (hydroxy) carbonate solid. Also influencing the chemical environment are portlandite and calcite, which are introduced into the repository both as cement in some of the waste forms and from the seal material used to close the shafts. In addition, commercial organic complexants (e.g., EDTA) already present in the waste could promote the dissolution and stabilization of actinides in solution. Iron present in the waste drums helps produce very reducing conditions but also may form corrosion products that could form colloids, which would sorb actinides. All of these potential interactions between the brine and the waste/backfill can have a significant impact on brine compositions and thus on mobile actinide concentrations.

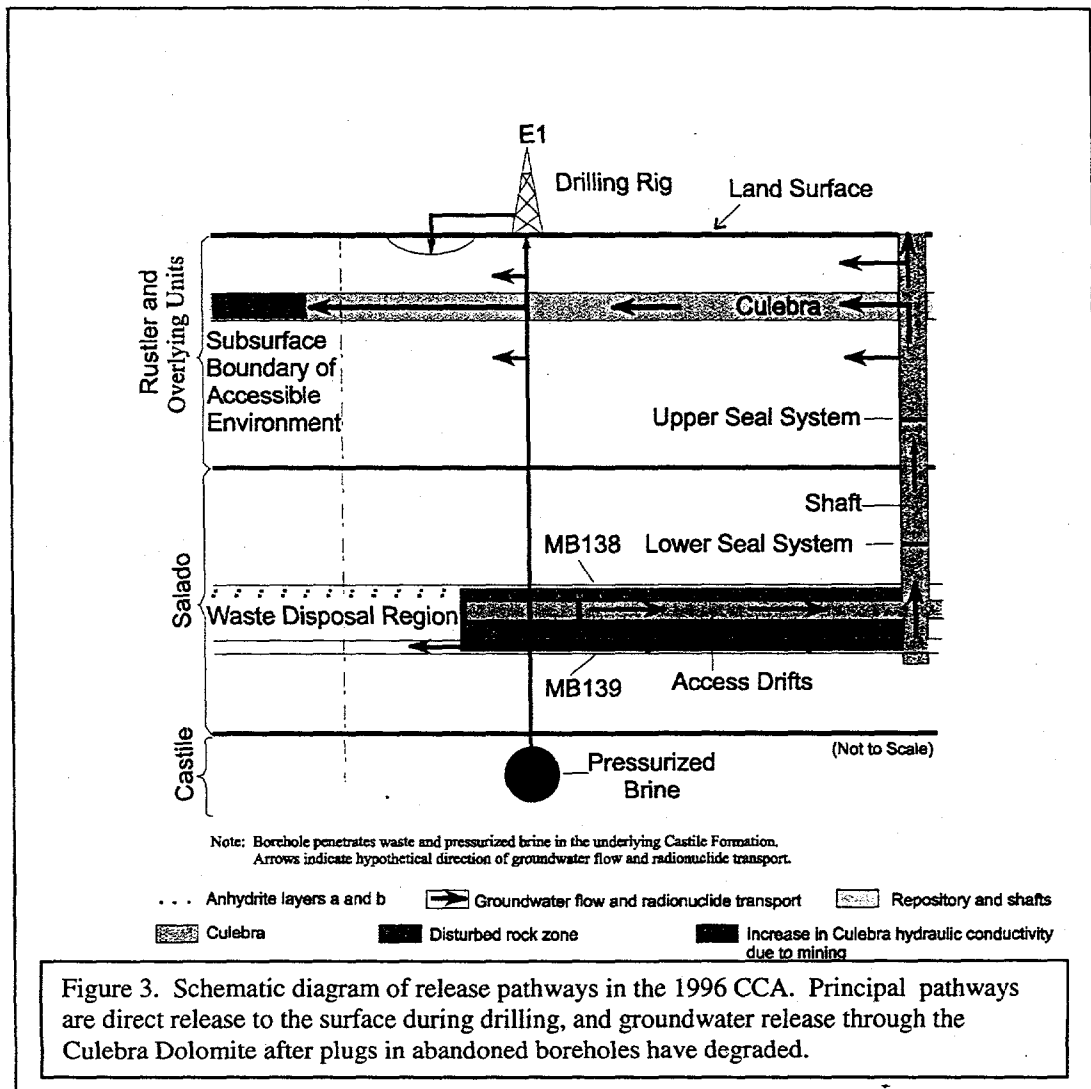
Both dissolved and colloidal actinides may contribute to mobile actinide concentrations. Dissolved actinides include hydrated ions, hydrolysis species, complexes with ligands, either inorganic, organic or both combined. Colloids are particles small enough to remain suspended in solution by Brownian motion, and are considered stable if they do not coagulate and/or settle out of solution by gravity. The processes governing the concentrations of mobile actinides include dissolution/precipitation, complexation with inorganic and organic ligands, formation and persistence of actinide-bearing colloids, and actinide adsorption. All of these mechanisms are fundamentally dependent on brine compositions. Colloid formation and persistence have an additional dependence on reaction kinetics and particle size. Adsorption will depend on the chemical nature of the substrate, regardless of whether the substrate is mobile or immobile.

The dissolved species model is based on the thermodynamic model developed by Harvie, Møller and Weare (HMW) [4]. The model utilizes a numerical algorithm that minimizes the change in the Gibbs free energy for the solution and relies on the Pitzer ion interaction formalism [5] to calculate activity coefficients in concentrated electrolyte solutions. This model is capable of describing most of the important chemical interactions in WIPP brines, including evaporite salt solubilities, potential waste or backfill additives such as calcium or magnesium oxides or hydroxides, and the carbon dioxide gas that may be generated within the disposal rooms. HMW developed a thermodynamic database, later extended by Felmy and Weare [6], which contains pertinent Pitzer interaction parameters to describe the chemistry of many natural brine systems. The model has been applied to the formation of borate mineral deposits, the determination of the compositions of Permian-age seawater and the evaporation of seawater. The HMW-FW model and data base have been extended by the WIPP actinide source term dissolved species program to include actinides and WIPP relevant organic ligands.

Colloidal particles are generally defined as particles with at least one dimension between 1 nm and 1 μm that are maintained in suspension in a liquid through Brownian motion [7]. Colloids can form by a variety of physical and chemical mechanisms including mineral fragmentation, intrinsic colloidal formation by actinides themselves or microbial degradation of cellulosic materials (e.g., humic acids). Additionally, microbes themselves may be considered to be colloidal particles because, though generally larger than the specified colloidal size range, their specific gravity is generally equal to the solution so they will not tend to settle out of solution by gravity. These four types of colloids – mineral fragments, actinide intrinsic, humic acids, and microbes – were each separately investigated as to their potential to enhance dissolved actinide concentrations and separate parameters for each type were submitted for the purposes of performance assessment.

Research indicated that both mineral fragments and actinide intrinsic colloids had little potential to enhance mobile dissolved actinide concentrations under the expected chemical conditions at the WIPP site. For PA, two parameters were used for the concentrations of actinides complexed by microbes and humic acids. The first parameters were proportionality constants representing the microbial and humic contributions to the actinide source term. These proportionality constants were multiplied by the dissolved species concentrations to obtain values for the microbial and humic contribution to the total species concentration. A second parameter was included to indicate a maximum value for complexation via these two colloidal mechanisms. Sorption of actinides onto fixed substrates in the waste disposal area was not considered because such sorption would not have an effect unless most of the actinide inventory were sorbed, which is considered unlikely.

The probabilistic PA conducted for the CCA predicts the performance of the WIPP disposal system over the next 10,000 years using computer models of the disposal system and random sampling of uncertain parameter values. Three hypothetical pathways were relevant to the mobile actinide source term: direct release to the surface during assumed drilling; groundwater release through narrow anhydrite interbeds in the Salado Formation (Marker Beds 138 and 139); and groundwater release through shallow aquifers (e.g., the Culebra Dolomite of the Rustler Formation) from movement of liquid up abandoned boreholes assumed to intersect the repository (Figure 3). The PA mobile actinide source term considers total aqueous actinide concentration to be the sum of dissolved and colloidal actinides. Random sampling of the concentrations over a 3.4 order of magnitude range was used to address uncertainty. In each vector in the suite of realizations, mobile actinide concentrations in the repository are held constant and equal to a random value within the range of uncertainty.



Lesson 1: Evolve Experiments and Performance Assessment Together

The WIPP actinide release scenarios considered for regulatory PA involve hypothetical conditions such as the effects of boreholes intersecting the repository which cannot be tested directly. Other processes considered in the PA can be tested directly, such as gas generation due to metal corrosion or microbial degradation of cellulose, but their importance is difficult to evaluate in the laboratory due to the time scales involved and process interdependencies that control the availability of key reagents, such as water. The bottom line is that the time scale and range of hypothetical conditions considered in PA cause large uncertainties in the predicted composition of aqueous solutions in the repository. This uncertainty creates difficulty in setting up a program of experimental characterization of actinide concentrations. Experimental programs need PA for system-level context and planning guidance; PA needs experimental programs for process-level guidance, and overall credibility and defensibility. For these reasons it is important that PA and experimental programs evolve together, with neither activity completely dominating the other.

In one example, preliminary PA calculations demonstrate that actinide concentrations under unconstrained chemical conditions were high enough that predictions of performance might not meet regulatory standards. The experimental program conducted solubility modeling and determined that low carbonate concentrations and pH values around 9 decreased the risk of non-compliance due to a large source term. The system-level PA calculations and the experimental program's detailed characterization of the chemical conditions providing low solubility were essential to make and defend a relatively costly decision to add an MgO backfill to the waste disposal rooms.

Feedback from PA on consequences of mobile actinide concentration values to repository performance also provided estimates of relative importance of various colloidal actinide-containing species. Screening calculations showed that two kinds of colloids were not stable in the high ionic strength WIPP brines at high enough concentrations to impact WIPP performance.

Expected WIPP chemical conditions were also important in establishing the insignificance of some colloid types and including others in the source term model. Solubility and population or site density (for microbes and humics, respectively) models were coupled with actinide loading models to predict upper bounds for colloidal mobile actinide concentrations under WIPP-relevant chemical conditions. Early stability and solubility screening studies showed that mineral fragments and intrinsic actinide colloids (colloidal size precipitates of actinide hydroxy compounds) are not present at concentrations significant for WIPP performance assessment (determined with feedback from PA). Halophylic microbes that are viable in WIPP-relevant conditions were shown to contribute significantly to the mobile actinide source term. Humics carrying (complexed with) actinides were shown to be sufficiently soluble in concentrated brines and small enough to be treated as dissolved complexes in retardation and transport modeling.

The lesson learned is to use iterative loops between PA and experimental programs to understand the system-level effects on repository aqueous chemistry early; determine the range of possible actinide concentrations given the system-level uncertainties, and if necessary to tailor the backfill (or other performance-affecting additive) to control source-term chemistry to acceptable limits thereby holding actinide concentrations to acceptable levels.

Lesson 2: Chemical Processes are too Complex for Performance Assessment

The range of possible chemical conditions in the WIPP disposal room are too complex to be described exactly. In order to develop a tractable yet conservative performance assessment model for actinide solubility at WIPP, many simplifying assumptions had to be made. For estimating dissolved concentrations, these assumptions are: (1) complexation and precipitation/dissolution (non-redox) reactions can be described with equilibrium thermodynamics, (2) solubility will decrease with time as more stable actinide solids develop (i.e., predicted solubilities are conservative), and (3) actinide conversion between oxidation states (redox reactions) is not an equilibrium process.

The assumption of equilibrium for all non-redox reactions provides a great simplification in the description of the system and an additional measure of conservatism in the conceptual model. Implicit in this assumption is the corollary: "actinides in the waste dissolve immediately when contacted with brine," which is clearly conservative. However, determination of the kinetics of actinide dissolution for the actinides in WIPP wastes would require location and characterization of the actinides in the heterogeneous waste mixture, an exceptionally challenging task. The assumption of instantaneous dissolution obviates this problem, and yields higher concentrations of mobile actinides, particularly in the early years of repository life, which is conservative with respect to regulatory requirements.

The assumption of instantaneous equilibrium for non-redox reactions also implies that actinide solid phases will precipitate immediately when the brine is supersaturated. This corollary does not appear to be conservative, but this concern is mitigated by further consideration. The formation of actinide precipitates in the laboratory is typically examined over a time scale of days to months, which is effectively instantaneous when compared with the 10,000 year regulatory lifetime of the WIPP. The actinide solid phases included in the model are only those that have formed within the laboratory time frame. Many of these solid precipitates will be metastable and will convert to more stable forms as they age [8] with a corresponding decrease in solubility. Therefore, using laboratory-determined, possibly metastable, solids for the precipitated actinide phases is conservative.

Finally, the dissolved actinide conceptual model assumes that oxidation-reduction reactions are not considered to be at thermodynamic equilibrium. Oxidation-reduction equilibrium is often not attained in low temperature geochemical systems like the WIPP, even over geologic time [9]. The kinetics can be very slow, and conversion among oxidation states is strongly influenced by other factors. The WIPP disposal room environment will likely contain regions in which radiolysis would produce oxidizing conditions, regions in which large quantities of metallic iron will produce reducing environments, and regions where microbes may catalyze conversion among actinide oxidation states.

The conceptual model for the chemistry at the WIPP site attempts to describe the complex natural and artificial chemical conditions expected to influence dissolved actinide concentrations in the repository. By utilizing some assumptions regarding the reaction kinetics and interactions between the waste and the brines present at the repository, the WIPP system was simplified so that it could be manageably described by mathematical analyses. It was determined that an equilibrium thermodynamic model to evaluate actinide solubility in the WIPP brines would be both mathematically feasible and scientifically supportable.

The thermodynamic solubility models must describe the brine compositions resulting from interactions between Salado and Castile brines with the wastes and backfill. To simplify the experimental requirements for developing an actinide solubility model, an oxidation state analogy was employed which assumes similar behavior for all actinides in a particular oxidation state. This approach was essential when making predictions for Pu. Pu can exist in four oxidation states and a method for holding Pu solely in the IV and V states has not been found. Table 1 lists all species that will be present in the WIPP disposal room along

Species in WIPP	Representative Actinide (Solubility Upper Bound)
Pu(III), Am(III)	Am(III)
Th(IV), U(IV), Np(IV), Pu(IV)	Th(IV)
Np(V)	Np(V)
U(VI)	U(VI)

Table 1. Oxidation States Present in the WIPP and Analogous Actinide for Determining Concentration in WIPP Brines

with the representative actinide used in modeling. For example the solubility model for Am(III) was used to calculate solubilities for Am(III) and Pu(III). Each of the representative actinides give values that are solubility upper bounds for all of the actinides in that particular oxidation state. The use of oxidation state analogs is well documented [10,11,12,13]. The lesson learned is to design experimental program not only to understand processes that are expected to occur, but also to provide support for the types of simplifications that will be necessary because PA models cannot incorporate the complexity of fundamentally realistic chemical reaction models.

Lesson 3: Involve Experimentalists in Performance Assessment Simplification

In the WIPP project, few of the scientists who collect chemical data are directly involved in the development and application of system-level performance assessment calculations. Because thorough external review was expected, agreement between model developers and experimental scientists was critical and could not be left to chance. A managed process was used to ensure that the individuals responsible for model and parameter development included the viewpoint of experimental scientists. The steps in SNL's process were:

- Experimental chemists document data available, interpretation of data, and propose PA models and ranges of parameter values
- Experimental chemists and PA chemical modelers met to develop PA model, discussing key simplifications and implementation approach
- Later, experimental chemists, PA modelers, and data/uncertainty experts met and determined parameter range and probability distributions
- Internal review for consistency and completeness
- Final documentation of parameter ranges and distributions is prepared and archived in a formal records center.

The meetings on PA models and parameter distributions provided were used to address simplifications of the chemical system used in the PA models, such as the assumptions of homogeneity, equilibrium thermodynamics, and the use of the oxidation state analogy. Because documentation rather than trust is the basis of regulatory decision-making, a transparent record of these discussions and their results is critical in convincing the regulator and stakeholder of the credibility of the PA model.

Lesson 4: Incorporate External Peer Reviews Early and Often

Peer review is an essential part of sound science and engineering. All work should be reviewed by technical peers, and documentation of peer review following the concepts of traceability, transparency, retrievability, and reproducibility should be standard practice. Peer review may be internal or external, by individuals or panels. There are two basic types of peer review panels: Expert Review Panels and Formal Expert Elicitation Panels. Expert Judgement is the use of personal or team knowledge and experience to design, execute, and interpret experiments or build models. Expert elicitation is the use of external knowledge or experience to supplement information gathered internally by scientific investigations.

Expert peer review was used to build confidence in the acceptability and integrity of the mobile actinide source term program. It helped identify, prioritize and defend potential activities, and familiarize the scientific community with its details. Furthermore, it provided WIPP project chemists with insights into the types of questions to expect from outside scientific reviewers not familiar with the project. The incorporation of expert opinion into planning, implementation, and technical review of the mobile actinide source term research program is extensive. As an example, consider the WIPP Colloid Research Program, which was initiated in Fall 1992.

To help in planning the program, informal discussions were held in early 1993 with experts at several institutions, including the Colorado School of Mines, the University of Colorado, the California Institute of

Technology, the Lawrence Berkeley National Laboratory, the Lawrence Livermore National Laboratory, and the Los Alamos National Laboratory.

Based on information acquired from those informal discussions, and an extensive review of the literature, a preliminary planning document was prepared by Sandia National Laboratories and reviewed by experts from the California Institute of Technology, the Lawrence Berkeley National Laboratory, the Lawrence Livermore National Laboratory, Florida State University, the Pacific Northwest National Laboratory, the Colorado School of Mines, the Oak Ridge National Laboratory, and the University of Miami. Information compiled from those reviews, together with information gained from preliminary experiments conducted at Sandia National Laboratories and Lawrence Livermore National Laboratory were used to develop a detailed Test Plan [14].

The WIPP Colloid Research Program was conducted by specialists from several institutions, including: microbial colloids at Brookhaven National Laboratory; humic colloids at Florida State University, at Colorado School of Mines, and at Sandia National Laboratories; actinide intrinsic colloids at Lawrence Livermore National Laboratory; mineral colloids at Sandia National Laboratories; colloid transport experiments at Sandia National Laboratories; and transport modeling at SciRes and at Sandia National Laboratories. While the work conducted at these institutions was focussed on specific portions of the overall colloid research program (except for overall project management at Sandia), the researchers in all locations provided suggestions for other parts of the program.

Approximately half way through the research program, a day-long review was held and comments solicited from experts from the Colorado School of Mines and Galson Sciences Ltd. Quality Assurance assessments and formal reviews were conducted frequently at Sandia and at contractor sites.

The final results of WIPP Colloid Research Program were reviewed in Spring 1996 by the independent, EPA-mandated Conceptual Model Peer Review Panel, the National Academy of Sciences/National Research Council WIPP Panel, the New Mexico Environmental Evaluation Group, the New Mexico Attorney General's office, the DOE/Carlsbad Area Office, and expert consultants employed by those groups. Results have also been presented extensively at a variety of national and international technical meetings and published in significant journals requiring peer review. The lesson here is that external review conducted during the planning and implementation stages of an experimental program builds-in the confidence and documented evidence that will be required by later regulatory or stakeholder reviewers.

Discussion and Conclusion

WIPP's success in certifying the WIPP with EPA regulations required (in part) demonstrating through documentation that models of physical processes incorporated into the PA modeling system were credible and acceptable for predicting long-term performance. In developing the PA models and data bases for the mobile actinide source term, pragmatic lessons were learned are: (1) iterate between experimental programs and performance assessment calculations to prioritize experimental programs and model development activities; (2) target experimental programs not only at processes but also to support the simplifying assumptions that will need to be incorporated in PA models, (3) develop PA models and parameter values with strong involvement of experimental chemists; and (4) incorporate external peer review early and often, even in the planning and implementation stage. A cross-cutting lesson learned is that documentation through records is the basis of decision-making: accordingly, work must be traceable, transparent, reviewed, reproducible, and retrievable. Fundamentally, credibility depends on documented and retrievable records of work, consistency with standard scientific and engineering practices, and reasonable consideration of alternatives. It is hoped in sharing these lessons learned that other organizations pursuing deep geologic disposal will overcome tough challenges with less difficulty.

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