4.2.1. Heterogeneity and Model Discretization

Much recent hydrogeologic research has clarified the importance of heterogeneity in controlling solute transport. What constitutes an adequate scale of definition of formation heterogeneity for a flow model may be inadequate for solving the transport equation in the same formation. Konikow[21] presented results of numerical experiments indicating that the CCA consistently underpredicted the migration distance of a plume emanating from a human intrusion borehole. In the CCA model of the Culebra, it appears that errors arising from several sources cause an artificial spreading of the calculated width of the plume at the expense of its length. If the plume spreads out laterally more than would actually occur, for a given mass of contaminant released from a leaky borehole, the wider plume will necessarily move downgradient a shorter distance than the narrower plume. The sources of these errors include numerical dispersion and spatial truncation errors in the transport code, poor resolution from using a grid that is too coarse for the scale of the problem, and overestimates of the size of the solute source area.

The solute-transport model used in the CCA is based on a finite-difference grid having a minimum spacing of 50 m. An alternative analyses was performed using the MOC3D model[22] in which the transmissivity variations are represented on a much smaller scale, using a 2-m grid spacing rather than the original 50-m grid spacing. This finer scale representation of the heterogeneity and of the borehole source area results in a much longer, but narrower, plume that would have a significantly shorter travel time to the regulatory boundary for equivalent concentration levels.

4.2.2. Heterogeneity of Other Transport Parameters and Processes

The CCA model of the Culebra assumes that most properties of the system, except the transmissivity, are homogeneous and uniform within each simulation realization, but that these properties varied from run to run. Field tests at WIPP, however, indicate significant variability in many of these properties. For example, the effective porosity of the aquifer varies by almost an order of magnitude, even over a distance of only 50 m (the size of one cell of the model grid). Porosity has a strong control on transport velocities and times. Hence, the variability in porosity induces variability in velocity, which means that some parts of the plume may move faster than the local average velocity. This effect cannot be captured by assuming that porosity is uniform in each simulation. One would expect other properties, such as K_d and fracture spacing, to similarly exhibit large spatial variations. The PA procedure inherently assumes that heterogeneity in these variables has no significant impact on transport, or that its effects can be adequately represented by varying uniform properties among all the realizations. Either way, the CCA has not demonstrated that this is indeed the case and that it is reasonable to ignore the spatial variability in all of these critical parameters.

4.2.3. Sampling Procedures for Input Parameters

To generate the statistical distributions from which the risks are calculated, many simulations of hydrogeologic processes are performed to generate an adequate sample size. The approach to varying the values of the many parameters in the multiple realizations can introduce errors into the final analysis. In particular, if hydrogeologic variables that are highly correlated are sampled independently and if the correlations are ignored, then some of the realizations may be based on unreasonable or very unlikely combinations of parameters. Such individual simulations should not be incorporated into the final analysis because they may skew the statistical results. For example, the CCA separately sampled and independently varied aquifer transmissivity, fracture spacing, and porosity. Yet there is good reason to suspect that these variables are interrelated. The concern is that the net effect of independently sampling correlated parameters could yield a biased risk assessment, as described in more detail in Ref 8.

4.2.4. Consistency Between Performance Assessment (PA) Models

The PA procedure uses one model to calculate the fluid and solute flux up and out of a human intrusion (HI) borehole. This outflow flux should then be equal to the input flux (source term) in the Culebra model that is used to calculate transport distances and times. However, the source term in the Culebra flow model is apparently not represented as a specified fluid flux, so it is unclear that the flux out of the borehole is equal to the flux into the Culebra for each set of realizations (or even for the mean of all realizations). The PA models should compute mass balances and budgets, to demonstrate that the two boundary conditions are indeed equivalent. Specifically, the total mass of fluid and solute that the borehole model computes to enter the Culebra over 10,000 years should equal the total mass of fluid and solute that is added to the Culebra over 10,000 years in the Culebra model. It appears possible that representing the HI borehole solute flux as an initial condition in the transport equation without an accompanying fluid flux could lead to a consistent underestimate of the solute spreading away from the finite-difference cell where the HI borehole is assumed to be located.

4.2.5. Other Concerns About the Culebra Parameters and Processes

The NAS WIPP Committee report (Chapter 6 and Appendix F of Ref. 20) included a number of criticisms of the conceptual models and numerical models of the Culebra, many of which remain unresolved. The most critical issues relate to the use of homogeneous and uniform K_d values in each realization, and whether the very simple retardation factor concept adequately represents all of the complex reaction chemistry. This has certainly not been adequately demonstrated at the field scale. A related important issue is the accuracy of the definition of matrix diffusion processes and parameters. Another concern is the reliability of the regional transmissivity estimates for the Culebra, which were determined using inverse methods that assumed a nonleaky two-dimensional aquifer. Three-dimensional analyses by Sandia[23] clearly indicated that there is significant leakage into the Culebra. A Climate Index has been used as a multiplication factor in the CCA to enhance the magnitude of flow of the Culebra flow field to compensate for the lack of consideration of the additional flux through the system. However, we have not seen any rigorous analysis and documentation of the consequences of such errors, or the sufficiency of corrections applied.

4.2.6. Current Efforts to Resolve the Culebra Transport Issues

Many of the shortcomings listed above arise from the fact that the models developed for the flow and transport of radionuclides through the Culebra are computationally expensive to perform, i.e., have very long run times. Adding complexity from the suggested comments would only further increase these run times. To help combat the strain of additional development on transport calculations, a new 1D, semianalytical approach was taken on the latest round of sensitivity analyses.[23] The calculations used a particle tracking code to map out a series of curvilinear paths from the steady-state flow velocities, on which a 1D analytical transport calculation was performed. The calculations experienced decreased run times, with comparable results to the CCA. The results open the door for increased complexity and more realistic model assumptions.

In addition to the increased modeling effort, extensive laboratory and field investigations are being conducted to understand the diffusive nature of transport in the fractured media. Field tracer experiments suggest that breakthrough curves are best replicated with a dual-porosity, multi-rate diffusion model.

4.3. Chemical Retardation

The values for sorption coefficient K_d used in the PA impact the postulated releases of radionuclides through the Culebra pathway. Independent checks of the CCA calculations by the EPA and the EEG show that only a 3 ml/g value for K_d is sufficient for showing compliance with the containment requirement of the EPA standards (40 CFR 191.13). This conclusion relies on keeping all the other parameters and assumptions in the CCA unchanged. It is difficult to accept a particular value or a range of values for any of the input parameters on the basis of partial sensitivity analyses. To have confidence in the calculations, the values of all input parameters should be independently verifiable to be robust and based on valid experimental data. The EEG recommended[8] resolution of the following issues to justify properly the K_d values.

4.3.1. Limitations of Laboratory Data

The EEG has accepted the validity of using the laboratory-determined K_d values to get an estimate of the values to be used for modeling contaminant transport in the field because groundwater diffusion into the rock matrix will provide opportunities for chemical retardation to occur. This does not mean, however, that a one-to-one correspondence may be assumed between the laboratory and field values. The K_d range determined from batch tests applies only to the matrix porosity, and not to retardation in the fracture system with advective porosity.

4.3.2. Limited K_d Database

The experimental database for the K_d values used in the CCA remains insufficient. In the absence of measured K_d values for plutonium at oxidation states III and IV and inconclusive results for Am^{III} the K_d values for these three most important actinides in the WIPP inventory have had to be estimated. These estimations are based on two questionable assumptions. The first is that K_d values for actinide cations of the same charge should roughly be the same. The weakness of this assumption lies in not considering the effect of the speciation behavior of the cations on their adsorption properties. The second assumption is that predictable trends exist for the K_d values of actinide cations of different charge. The DOE used this assumption to argue that Pu^{V} data can be used for Am^{III}. This assumption is based on questionable data and interpretations of the experiments conducted with dilute groundwater from the Yucca Mountain site, even though, fortuitously, the same trend has been reported by some other experimenters. Results of the intact core column tests are probably of questionable value as well. The Am and Pu input concentrations to the cores were so close to saturation with solids that precipitation rather than adsorption may have occurred.

The net result of these assumptions is the use of unjustified K_d values for the three most dominant radionuclides in the WIPP inventory. Pu^{V} data have been used for Pu^{III} through a two-step process, both of which are questionable: first, through the predictable trend argument for Am^{III}, and then through the oxidation state analogy for Pu^{III}. Similarly, Th^{IV} data have been used for Pu^{IV}.

The oxidation state analogy is most useful as a starting point for designing an appropriate experiment, but the answer is not known until the experimental measurement is actually determined. As stated in the NAS/NRC WIPP Committee report, "Although the oxidation state model (the assumption that the chemistry of a given oxidation state is similar for all of the actinides) is an appropriate beginning to a difficult problem, deviation for the oxidation state analogy are well known in natural and experimental systems. Substantial experimental verification will be needed to establish the limits of this analogy."[20]

Besides the inherent limitations of the oxidation state analogy, there is an additional problem of an inapplicable brine (from ERDA-6 brine reservoir) having been used for the Th^{IV} experiments. The mean K_d values measured in the ERDA-6 brine are greater than the values determined using the WIPP repository brines.

4.3.3. Use of Laboratory Data

The EEG expressed concern[8] with the CCA values for the lower and upper bounds of the K_d probability distribution and how these bounds are defined relative to the type of brine used in the batch experiments. The ranges for K_d relative to brine type were selected based on the average value of the sample distribution. For example, the range for Pu^{V} (and by extrapolation, for Pu^{III} and Am^{III}) used in the CCA calculations is 20–500 ml/g, which reflects values from the batch tests using deep brines. The lowest K_d value using the Culebra brine was 9.8. The assumed range for Pu^{V} should have been 9.8–500 ml/g.

4.4. Solubility of Actinides

The solubility of actinides is very important in calculating releases from the repository. The FMT model used in the CCA predicts differences for actinide sulfate solubilities that cannot be explained by chemistry, thus raising questions about the reliability of this model. DOE is considering replacement of the FMT code with EQ3/6 for the first recertification.[25,26]

Rather than using an extensive plutonium database, the FMT predictions relied on thermodynamic data for other elements and an oxidation state analog argument. EEG recommends that the calculations be performed using thermodynamic data for plutonium.

The CCA discounts the role of organic ligands on plutonium solubility. It argues that the entire repository waste is a homogeneous blend and that the chelating compound EDTA is the strongest complexing agent and the amount of it present in the inventory is not enough to make a difference. But citrate forms stronger complexes with actinides in the +IV oxidation state than with other cations. The solubility of a stable plutonium–citrate complex in individual waste containers needs to be determined.

Plutonium constitutes 82% of the radionuclide inventory of the repository. The PA efforts of 1991 and 1992 attempted to capture the effects of oxidation state on solubility throughout the full range of the four possible oxidation states for plutonium in the repository: III, IV, V, and VI. To the contrary, the 1996 PA was based on calculations which assumed that the iron in the repository would force a reducing environment, thus allowing only Pu^{III} or Pu^{IV}; there would be no Pu^{V} or Pu^{VI} which can have higher solubilities. However, some of the experimental results from the Source Term Test Program, with liters and drums of TRU waste, show very high solubilities, suggesting the existence of either Pu^{V} or Pu^{VI} despite the presence of iron. The observation tends to undermine the assumption that all plutonium will be in either oxidation state III or IV. This issue needs to be resolved.

4.5. Direct Release Through Human Intrusion

As one of the dominant modes of release, a valid model for the spall of waste into an intrusive borehole is needed. Spall is waste that has been introduced into the drilling fluid due to radially channeled, highly pressurized gas flow from within the repository to a lower pressure borehole. The conceptual model peer review[27] found the spall model initially proposed by DOE to be conceptually inadequate. The DOE schedule for submittal of the application left insufficient time for development of an appropriate model. The DOE provided the panel with additional experimental information and results from other modeling efforts and asked the panel to consider whether the spalling volumes predicted by the original inadequate model was acceptable for use in the PA. It was argued by the DOE that the inaccurate predictions were acceptable because the predictions overestimated the release during a spall event. The peer review group accepted the inaccurate model based on that argument.[28] After DOE submitted additional information, EPA also accepted the model results for the purposes of PA.

The overestimated prediction stems from the development of an additional model for release calculations. This new model predicted releases about 1/20 of the original calculations, thus leaving the impression that the original model made a conservative prediction. However, both are inadequate and hence it is unknown which model's prediction is closer to reality. Testing of the new model[8,9] revealed serious instability problems outside a narrow range of waste permeabilities as shown in Fig. 5. For the waste strengths investigated there can be no confidence in waste permeabilities outside the narrow range of 1.7 to 2.0×10^{-13} m².

The EPA maintains that the code behaves quite reasonably under expected repository conditions. Assuming "expected conditions" is suspect given the uncertainty that arises from the geologic and hydrogeologic response of the repository system, along with the gas generation from the degrading waste. The fundamental philosophy behind the PA is to sample the input parameters from an expected range. To state that one set of conditions, for which the model is applicable, correctly captures all uncertainty inherent in long-term modeling underestimates the importance of accommodating such uncertainty. A new approach is needed to develop a coherent and straightforward model to address the important issue of spall supported by a suite of appropriately designed experiments by which to determine waste strength.

As a part of the recertification effort by DOE, work is in progress to capture adequately the physics of spall in a new model. The new model will incorporate a modified wellbore hydraulics model with mixing equations for solids and fluids, a drillbit damage

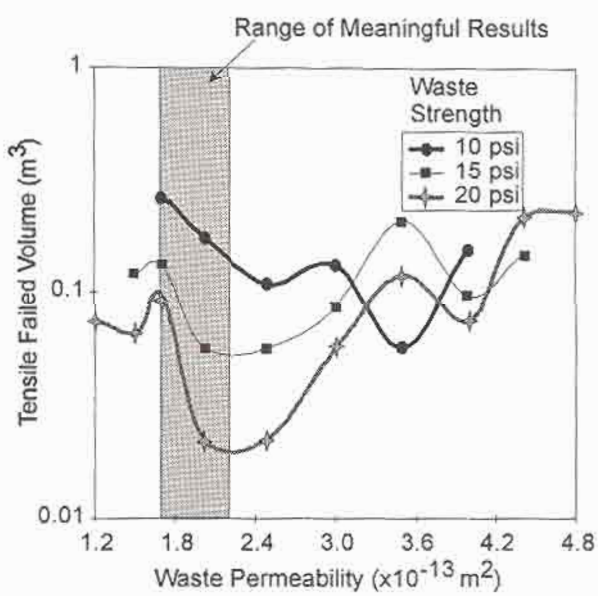

Fig. 5. Tensile failed volume from GASOUT predictions for various waste strengths and waste permeabilities.

model, and a solids transport up the borehole annulus. Previous models assumed that all of the material that failed in the bottom of the borehole would be transported to the surface. However, by actually modeling the phenomenon, the likely result would be that only a fraction of the material would reach the surface and reduce the overall effects of spallings on the CCDFs.

4.6. Fluid Injection

Brine injection for saltwater disposal and enhanced oil recovery is already underway near the WIPP and throughout the Delaware Basin.[29,30] The history of water migrating away from leaking injection wells through the Salado Formation in southeast New Mexico is well documented.[30–32] Nonetheless, fluid injection for oil recovery within the designated WIPP boundary was not included in the 1996 performance assessment calculations. The DOE rejected the scenario on the basis that the EPA regulations did not require it. Only the drilling event was included.

The first step in a performance assessment is to screen features, events, and processes (FEP). Two grounds for rejecting a relevant scenario from consideration in the PA calculations are low probability or low consequence. Probability and consequence, however, are not considered if a scenario has already been eliminated on the basis of regulation. The regulation states: "With respect to future drilling events, performance assessments need not analyze the effects of techniques used for resource recovery subsequent to the drilling of the borehole."[3]

The regulation does not preclude DOE from including the fluid injection scenario as part of the recertification effort. In some instances, the EPA certification identifies the need to further evaluate a scenario that was eliminated on the basis of regulation. For example, the EPA determined that DOE did not need to include air drilling in the PA because it was not a current practice and thus it was ruled out on the basis of regulation. Nonetheless, EPA conducted further analysis "solely to allay the public's concern"[4] on the issue. Given the presence of oil reserves, the probability of future drilling, and the reasonable expectation that the reserves will be recovered by methods including fluid injection, it would seem prudent for the recertification effort to revisit the issue of fluid injection within the WIPP site boundary.

The OECD/NEA–IAEA Joint International Review Group also expressed reservations about rejecting a scenario solely on the basis of regulatory considerations: "It would improve the confidence of the reader if the DOE presented the logical or physical arguments for not considering these processes in the assessment, in addition to noting that they are not required in a compliance demonstration. Otherwise, there is an impression that processes that might deserve consideration from a safety perspective have been eliminated."[33]

Recertification can also incorporate new information from the expanding fluid injection practices surrounding the WIPP site. The effects of leaking injection wells adjacent to the site were screened out from the performance assessment calculations on the basis of low consequence by the DOE[1] and low probability by the EPA.[4] The DOE had chosen to examine consequence rather than probability, recognizing that certain petroleum practices are hard to define in a probabilistic sense.[34]

The EPA Certification relies on the DOE's low-consequence argument as the basis for rejecting fluid injection as a scenario.[4] However, the EPA acknowledges that certain scenarios can be constructed that inject large volumes of fluid into the repository. In these cases, EPA relies on its own probability calculation to screen out certain combinations of natural and human events (pp. 24–25 of Ref. 35).

The EPA multiplied the probability of each event to determine the probability of an injection well impacting the repository. Initially, EPA determined the probability of an injection well impacting the repository as 1 in 667 million (Table Q of Ref. 36), a value which was widely cited by others (p. 111 of Ref. 8; p. 45 of Ref. 37; p. 27 of Ref. 38). The final technical support document maintains that the original value was 1 in 58,000.[39] Based on new estimates of individual events, the probability of a leaking well impacting on the repository was then estimated to be 1 in 171,000.[4] Thus, the EPA analysis advanced three different values of probability, spanning four orders of magnitude. The uncertainty lends support to the DOE position that it would be difficult to defend the probability argument because it would be difficult to define the performance of individual components in a probabilistic sense.[34]

In summary, recertification should consider the effect of fluid injection just outside the site to accommodate the reasonable expectation that there will be an effort to produce the crude oil reserves by waterflooding and there will be saltwater disposal of produced brines. The recertification also needs to examine developing information from the saltwater disposal, oil field pressure maintenance, and oil field waterflooding activities adjacent to the WIPP for inclusion into future PA calculations. Just as a scenario can be screened out, a scenario can also be screened in, based on new information or a reexamination of existing information.

4.7. Solution Mining

The one impact of potash mining that has been considered in the CCA is the alteration of the transmissivity of the overlying Culebra aquifer as a result of subsidence due to conventional mining. The EPA argues that near-future activities, such as solution mining for potash, can be eliminated on the basis that it is not now occurring in the Delaware Basin and to assume its occurrence in the future would be speculative. Nonetheless, solution mining is a proven technology that has near-future potential. The EPA criteria require consideration of near-future activities. The EPA guidance specifies that this includes plans for new mines in the vicinity of WIPP.(40)

By delaying the development of oil and gas reserves surrounding the WIPP (Fig. 3), the U.S. Bureau of Land Management has indicated its plans to first allow the mining of the potash. Meanwhile, the New Mexico Bureau of Mines and Mineral Resources,(41) at the request of DOE, identified one feasible future technique for potash recovery—solution mining of the remaining sylvite reserves. The report notes, "all mines have held open the option of using solution mining once their sylvite deposits are fully mined out."(41)

With the continued production of potash, PA needs to screen plausible scenarios with each recertification. The actual impact on the transmissivity of the overlying aquifers needs to be monitored. At this time the PA calculations rely on estimating the range of modification to the transmissivity of the Culebra aquifer. Changes in the transmissivity are multiplied by a factor sampled from a range of 1 to 1,000. As potash mining continues, it would be worthwhile to obtain a measurement of the change in the transmissivity to determine if this range is appropriate. In addition, other parameters, such as fracture density and aperture, diffusion, and dispersion, should be accommodated during a subsidence event.

4.8. Engineered Barrier

Like the spall model, the use of MgO backfill was another late development in the performance assessment that proved troublesome during the conceptual model peer review(27) and later during the EPA rule-making. Rather than decrease uncertainty in the calculated performance of the repository, the addition of MgO may increase uncertainty. First, there is no consensus on the behavior of the system. Experiments with MgO showed that various mineral phases would form, but nesquehonite was the only mineral phase that could be identified. It is also not known how long the nesquehonite phase would persist. For purposes of certification, the EPA accepted the initial DOE argument that the nesquehonite would be short-lived and the system would be dominated by other mineral phases. To further complicate the issue, the DOE later argued that the nesquehonite would never form under repository conditions.(37) The solubility model used in the 1996 PA calculated a substantial increase in plutonium solubility due to the presence of nesquehonite. EEG's calculations with the performance assessment model shows that while such a solubility does not result in a violation of the release limits, there is very little margin for error.(9)

5. RECOMMENDATIONS

Future iterations of performance assessment, as part of each recertification, need to consider the following recommendations.

1. The available data strongly suggests a 60% probability of drilling into a high-pressure brine and this value should be used for PA calculations.
2. The use of grid refinement for transport through the Culebra should be thoroughly explored and rigorously tested. Moreover, the effects of the heterogeneity of parameters, such as porosity and retardation, should be captured.
3. Chemical retardation values should be experimentally determined for the actinides of interest.
4. The actinide solubility of plutonium should be based on thermodynamic data for plutonium.
5. The spalling model needs to reflect the results of a carefully designed experimental program

to determine waste strength and a workable conceptual and numerical model.

6. Each recertification will need to consider new information from resource recovery activities, such as fluid injection and solution mining, as part of the first step in PA scenario development.
7. The behavior of the only engineered barrier, magnesium oxide, needs to be experimentally determined.

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Section 4.2 of this paper contains a summary of concerns brought to the EEG's attention by Dr. Leonard Konikow of the U.S. Geological Survey. Dr. Konikow developed these concerns while he served on the National Academy of Sciences WIPP Committee from 1989 to 1996. These were sent to L.C. as personal communication in February 1998. These issues are described in detail in Section 2.9 of Ref. 8 (EEG-68). The authors are also grateful to Dr. Jon C. Helton for providing an informal review of the paper.

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40. U.S. Environmental Protection Agency, Office of Radiation and Indoor Air, Compliance Application Guidance for 40 CFR Part 194, EPA 402-R-95-014 (1996).
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