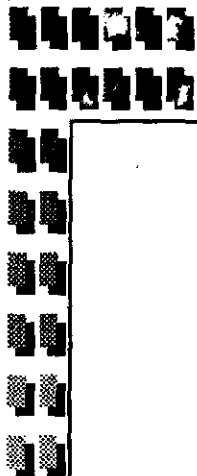**Sandia National Laboratories**

Waste Isolation Pilot Plant

Conceptual Models Information

for

The Peer Review Panel

WIPP:1.5.1:PER:NQ:510788

Supplemental Information

on Conceptual Models

Presented in Section 6.4

of the

Compliance Certification Application

CONTENTS

**Historical
Development**

Historical Development of WIPP Conceptual Models

Ideas about the processes important to the performance of the Waste Isolation Pilot Plant (WIPP) have changed since the WIPP Project's inception in the early 1970s, as the U.S. Department of Energy (DOE) and its precursor agencies refined knowledge and understanding of features of the site and the processes and events that might occur there. Although the understanding of the WIPP site has continuously evolved since the early 1970s, the fundamental conceptual models that shaped projections of WIPP's performance underwent major changes only three times: in the mid-1970s during site selection; in the late 1970s during surface-based site characterization; and again in the mid-to-late 1980s during site development. Since the late 1980s, the fundamental conceptual model that shapes the current evaluations of the performance of the repository has not changed in any major way. Rather, experimental activities since the late 1980s have led to the level of understanding of the details of processes expected to occur at WIPP that is necessary in quantitative, probabilistic performance assessments. This section describes the evolution of the most-accepted understanding among WIPP Project staff of the processes and events of potential importance at the WIPP, without attempting to comprehensively list all the ideas considered at various times by WIPP Project staff or other interested parties.

Just as concepts about the important features and processes at the WIPP have changed as the project matured, so also have the techniques used to evaluate the consequences of radionuclide release from the repository changed. Changing the methods used to address the consequences of radionuclide exposure pathways has affected both the types of computational modeling used to evaluate performance and perceptions of the relative importance of the many physical properties of the disposal system. Until 1985, when U.S. Environmental Protection Agency (EPA) promulgated its standard for transuranic waste repositories, 40 CFR 191, the consequences of release were primarily evaluated in terms of human exposure to radionuclides that had reached the biosphere by some mechanism. Contaminant transport in the geosphere was not regarded as a problem if humans were not exposed. Two principle pathways were of concern. Direct releases to the surface from a borehole (cuttings, cavings, spallings, and brine flow in the present modeling system) could expose drillers and hypothetical future residents of the region who consumed livestock grazed nearby. Individuals could also be exposed by drinking water from a contaminated source or by eating livestock watered at a contaminated stock pond. For example, the hypothetical "Malaga Man" was one who drank water and ate fish from the Pecos River near Malaga Bend, a discharge point for contaminated ground water from the Rustler Formation. (The release of contaminated Rustler ground water at Malaga Bend is no longer considered plausible). The consequences of release by divers transport pathways were treated deterministically and individually. The time period considered for evaluating the effectiveness of WIPP was usually about a quarter of a million years, roughly ten half lives of plutonium-239.

With the 1985 promulgation of 40 CFR 191, which set release limits at defined boundaries, determining the possible contamination of the Pecos River or other areas far from the repository was no longer an objective of the consequence modeling. Rather, the total quantity of actinides released from the disposal system, a defined volume, became the primary measure for assessing performance, although dose calculations to humans were still of interest to many groups and

required for certain circumstances. The probabilistic methodology suggested in 40 CFR 191 led to an appreciation of the possible interactions among multiple boreholes, assessment of the probabilities of defined events, and formal assessment of the impact of uncertainty on estimates of physical quantities. The standard also established a regulatory time period, during which actinide transport and system performance must be modeled, of 10,000 years. The EPA regulations have become increasingly prescriptive about how the WIPP Project should incorporate the uncertainty associated with projecting human actions into the future into performance assessments. Increased regulation and increased familiarity with the site have gradually escalated expectations about the quantity and quality of supporting information used to support analyses of repository performance.

Interactions between the WIPP Project and outside groups have played an important role in developing the current understanding of the site. Interactions with the National Academy of Science for the duration of the project and with its WIPP oversight panel beginning in 1978 and interactions with the New Mexico Environmental Evaluation Group (EEG), created in 1979, have been the most important of these. Interactions with the State of New Mexico, particularly with respect to RCRA issues, and with the EPA, especially in recent years, have also contributed to the Project. At various times through the years, the WIPP Project has convened expert panels and working groups to obtain advice on certain issues; for example, an expert working group met for many years to advise on the treatment of uncertainty in characterizing the Culebra Dolomite Member of the Rustler Formation.

Conceptual Models Used During Site Selection (1975-1976). The Oak Ridge National Laboratory (ORNL) selected the site for WIPP in the early 1970s. At that time, the concept of long-term performance of the WIPP was based on an understanding that bedded salt deposits were dry, natural creep of the salt would encapsulate waste, salt had good heat-dissipation properties, and the northern Delaware Basin had predictable geology that was amenable both to repository construction and to predictions of performance. Site-selection criteria were strongly influenced by experience at the abandoned bedded-salt site near Lyons, Kansas, and consequently focused strongly on isolating the repository from potential breach mechanisms associated with resource exploitation and dissolution. Accordingly, buffer zones of two miles between the site and existing deep boreholes and of five miles between the site and any potash mining were established as criteria for siting, and interest in fluid flow in aquifers and abandoned boreholes was chiefly related to its potential for dissolving salt in the Salado Formation.

During site selection in the early 1970s, several ideas about the Salado Fm. and processes associated with radioactive waste disposal in it were accepted as facts. The formation was known to contain anhydrite layers; the Project wanted to choose a repository horizon without anhydrite beds in close proximity because they would interfere with creep and waste encapsulation. Project staff recognized that a disturbed rock zone (DRZ) would develop around the repository; but because of salt creep, the long-term effects of the DRZ were assumed to be negligible as the waste was encapsulated and the disturbed salt healed (i.e., as its properties became similar once again to those of intact salt). The generation of gas by microbial degradation of waste constituents was recognized as a possible pressure-building mechanism. Because the Salado Fm. was thought to be dry, corrosion of steel in the waste was not considered

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to be important. It was known that intra-granular brine inclusions could migrate toward waste due to the thermal effects of heat-emitting waste. This was of considerable concern because at the time it was intended that WIPP would have two excavations for waste disposal, one at a shallower horizon for relatively cold TRU waste and one at a deeper horizon for heat-emitting high-level waste.

The ORNL identified a candidate site northeast of the present WIPP site in 1974. As discussed in Chapter 2 and Appendix GCR, drilling of ERDA-6 in 1974 at that site revealed steeply dipping beds, missing units, and brine containing hydrogen sulfide near the deeper planned repository depths. The dipping beds and missing units indicated that a level, minable repository horizon free of anhydrite could not be expected. Hydrogen sulfide in the brine posed a potential hazard to mine workers. Thus, the discovery of the deformed beds and associated brine at the ORNL site changed the concept of uniform evaporite stratigraphy throughout the northern Delaware basin.

The ORNL site was deemed unacceptable, and a search for a new site with acceptable conditions was initiated in late 1975. The new search was conducted by Sandia National Laboratories (SNL). SNL used selection criteria similar to ORNL's, but allowed mining to be in closer proximity since solution mining was not a concern as it was at Lyons, Kansas. The present site was identified in December 1975. Examination of petroleum exploration data, primarily seismic reflection surveys, indicated that deformation was limited largely to a zone paralleling the buried Capitan reef. A region in which Castile deformation is absent was identified and borehole ERDA-9 was drilled near the center of the proposed site, confirming that the beds were flat-lying and that no brine was present at or immediately below the potential repository elevations. Consequently, because the site satisfied other criteria, it was accepted as suitable in 1976, and site characterization began.

At the end of site selection with the current site identified, the following concepts were accepted by the WIPP Project and shaped thinking about the consequences of repository development:
- the Salado was "dry," with no mobile intergranular liquid;
- intra-granular fluid inclusions could migrate in thermal fields;
- gas could be generated by microbial action;
- salt would creep and encapsulate waste;
- there are deformed areas and brine-producing areas in the Delaware Basin evaporites, but the present site was free of deformation and brine at the potential repository horizons;
- natural dissolution fronts would not threaten the repository for more than 250,000 years.

Conceptual Models Developed During Site Characterization and Repository Design (1976-1981). Experimental activities conducted at the site immediately after site selection focused on characterizing the encapsulation properties of the Salado Fm., the migration of intra-granular brine in a thermal gradient, microbial gas generation, and the hydrologic properties of aquifers above the Salado.

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After site selection, interest in fluid flow in water-bearing units of the area shifted from its effects on dissolution to the role of these units as potential pathways for radionuclide release. The Magenta and Culebra Dolomite Members of the Rustler Fm. and the Rustler-Salado contact zone were recognized from regional experience to be potential pathways. At the time, the relative importance of these units was unknown, so the first tests targeted all three. The Rustler-Salado contact did not yield significant quantities of water at the site and did not represent a significant pathway for fluid movement for either radionuclide transport or dissolution. The Culebra was more transmissive than the Magenta, and the transmissivities of these units varied by several orders of magnitude over the area of the site. In time, characterization of ground-water pathways for radionuclide release became the principal characterization activity pursued at the WIPP site.

The hydrologic properties of the Salado Fm. were characterized by surface testing (drill-stem tests) during this period. These tests indicated measurable permeabilities over substantial thicknesses of the Salado, suggesting that the permeability of the Salado was sufficiently high that gas generated by microbial action would dissipate into the rock without reaching high pressure. Accordingly, the program to characterize gas generation, which had been progressing through the late 1970s, was canceled.

Many repository breach mechanisms by natural processes were postulated during this period, and investigations began to evaluate their likelihood and consequences. These investigations examined volcanism, tectonism, karst hydrology, deep dissolution, and other processes. In time, all such naturally-occurring processes for breaching the repository were resolved as not likely to occur or not likely to occur in a manner that would impair WIPP performance.

Repository Design. The design of the repository—the dimensions and geometry of the rooms, pillars, and accessways—was conducted by Bechtel, Inc., in the late 1970s. The design sought to ensure long-term encapsulation of the waste by salt creep and to provide enough volume to dispose of the projected 6.2 million cubic feet of waste. Given these performance criteria, the physical dimensions of the repository were determined with primary consideration given to mine safety during waste-disposal operations. Because the repository was designed prior to underground access, the basis for the design drew on experience gained from potash mines in the Delaware Basin.

The initial repository design placed the shafts at the south end of the repository, an area for experimental activities north of the shafts, and the waste disposal region north of the experimental area. From early on, the DOE viewed the WIPP as a research and developmental facility that would conduct experiments that were of interest to a wide variety of disposal programs and concepts. Accordingly, the original purpose of the experimental area was to house experiments to support development of models of rock mechanics and salt creep, experiments on seal behavior, and experiments of interest to high-level waste disposal concepts, such as canister design and fluid-inclusion brine movement. It was not intended at first that the experimental region would support studies of phenomena that had been previously characterized from the surface, such as the permeability of the Salado Fm.

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The repository design did not intially include constructed barriers to separate the waste into modules. Early discussions with the NAS oversight panel led to concern that fire in combustible portions of the waste could pose a hazard to mine workers. Modularization of the waste was proposed to enhance mine safety. Because constructing closures is expensive and time-consuming, separating waste at the panel scale was seen as best of several options for balancing concerns about safety, cost, and mine operations.

In November 1981, the WIPP-12 borehole was deepened into the Castile Fm. and encountered large quantities of brine that flowed freely into the borehole and to the surface. The discovery of a Castile brine reservoir at WIPP-12 prompted the rotation of the waste panels from their planned location north of the experimental area to south of the shafts, the current configuration, and eventually led to a geophysical program in the 1980s to investigate the possibility of brine reservoirs under the panels. Both the DOE and EEG conducted consequence analyses of a drilling encounter with a brine reservoir like that at WIPP-12 and concluded that the health consequences were minor.

In 1980, Congressional legislation limited WIPP to the disposal of TRU waste, and plans for a spent-fuel disposal level in the Infra-Cowden salt near the base of the Salado were abandoned. Because TRU waste generates relatively little heat, migration of brine in fluid inclusions was of little concern for the WIPP after 1980, although tests were conducted of this phenomena because of continued interest in high-level-waste disposal in salt beds elsewhere.

Thus prior to underground access at the WIPP in the early 1980s, several conceptual models shaped the thinking about the performance of the WIPP repository:
- the Salado is dry;
- inter-granular fluid inclusions are unimportant;
- the Salado has permeability high enough that gas generated by microbial action will dissipate, and pressure will not build up;
- fluid flow and transport of radionuclides in Salado are negligible;
- natural processes are not likely to release radionuclides;
- the Culebra is most important upper aquifer;
- the Culebra hydrology is relatively simple;
- retardation in Culebra is assumed;
- WIPP-12 leads to rotation of panels away from encountered brine reservoir.

Conceptual Models Developed During Site Characterization and Development. The repository horizon was selected in 1982 after the initial shaft was sunk and after design of the repository had been established. The horizon was selected based on the preliminary design of the repository and on the need for an adequate thickness of salt above and below the excavation and anhydrite beds for effective encapsulation and ease of mining. The Project wanted the mine be at least 300 feet below the McNutt Potash Member to provide isolation from possible mining, wanted anhydrite bed or clay seams within the back (roof) be at least two to three feet above the repository to reduce the possibility of roof fall, and wanted the mine to be as shallow as possible

to lower costs. The horizon selected between Marker Bed 138 and Marker Bed 139 was deemed to best satisfy all criteria.

Immediately upon access to the underground, experiments began to investigate rock mechanics and salt creep. Experiments also soon began to investigate phenomena of interest to other waste-disposal programs, e.g., thermal effects, fluid-inclusion migration, and gas generation in canisters proposed for other sites. However, by the mid-1980s brine was seeping into the repository in the absence of thermal gradients. Brine dripped from boreholes drilled upward into the back and collected in downward boreholes. This surprised Project staff and eventually led to the most significant changes in the conceptual models of WIPP performance since the northern Delaware Basin was identified as a likely location for a repository.

The first concern raised by critics of the Project was that the waste would not become encapsulated in a solid mass by salt creep, because brine that had seeped in would impede such consolidation. The waste was envisioned to become fluidized in a brine slurry that could be ejected from the disposal horizon if penetrated by a borehole. Before long, information about the rate of brine inflow showed that the concern about a brine slurry was unrealistic because consolidation to a sufficiently low porosity would occur before significant amounts of brine could accumulate. However, a new series of tests was executed to validate beliefs about the hydraulic properties of the Salado that had been based on surface-based testing conducted in the late 1970s. These series of tests included the Small-Scale Brine Inflow, BSEP, Room Q, and in-situ permeability tests and laboratory flow tests. Some of these test programs continued until 1995. The tests revealed that the permeability estimates from surface testing were misleading: the actual permeabilities are much lower than first assumed, and the assumption of no mobile intergranular fluid in the Salado was not realistic.

The in-situ permeability tests showed that inter-granular fluids were involved in flow but also demonstrated that the drill-stem tests conducted in the 1970s had overestimated the permeability of the Salado Fm. This led to realization in the late 1980s that gas dissipation in the Salado would not be sufficient to avoid the potential for high pressures. Brine seepage into the repository raised the possibility of gas generation by corrosion of steel. In response to the newly recognized importance of gas generation, a new program to characterize gas generation began in the late 1980s.

Because of gas generation and low permeabilities in the far-field Salado, it was thought that high pressure in the repository could induce the Salado Fm. to fracture. This topic had been of concern in the 1970s before the gas generation program was canceled. The renewed concern about Salado fracturing led to a program to investigate hydrofracturing of the Salado by high pressures, and eventually to the adoption of a fracturing model in performance assessment.

Borehole penetration of the repository and resultant release of radionuclides directly to the surface, always considered a possibility, was treated deterministically in early evaluations of long-term performance. In the late 1980s, the borehole intrusion idea became more complicated. The promulgation of 40 CFR 191 made it necessary to consider the possibility of multiple boreholes and their interactions. The appreciation of brine saturation in the repository and

possible high gas pressures led eventually to two new postulated release mechanisms—gas spallation and brine flow during drilling—in addition to the cuttings and cavings releases that had been modeled previously.

Actinide solubilities were not considered important until the mid-to-late 1980s. Prior to this time, the WIPP Project's expectation that the repository would be dry made aqueous concentrations seem unimportant. From early on, the Project had considered adding getters to the repository (materials that act to remove radionuclides), not so much to control actinide mobility as to assure performance. From the mid-to-late 1980s, however, the importance of actinide solubilities has been increasingly recognized in conjunction with the identification and rising importance of release pathways involving fluid flow from the repository. The addition of getters to the repository has lost favor because direct control of solubilities by engineering the chemical conditions in the repository is more demonstrably effective than getters, and because economical geologic materials that act as getters (e.g., phosphates) generally are naturally radioactive, complicating their emplacement.

Transport of actinides in colloidal forms was recognized as potentially important by the late 1980s, and some allowance for their possible impact was made in the ranges chosen for actinide solubilities in early performance assessments. The effect of transport of actinides in colloidal forms was not explicitly modeled until the calculations for this application.

From the time of the initial conceptual design and the 1980 Environmental Impact Statement (EIS) it was assumed that backfill would be emplaced in the repository to help fill the void space and reduce the magnitude of subsidence in overlying units. This assumption was challenged in the late 1980s by calculations indicating that backfill would not significantly affect the overall subsidence above the repository. For a time, backfill was therefore not considered as part of the baseline design for the repository. Recently, however, the addition of a carefully designed backfill to control chemical conditions in the repository has been shown to have significant benefit in assuring lower actinide solubilities.

As the possibility of high gas pressure in the repository and the associated possibility of fracturing of the Salado re-emerged in the late 1980s, it became apparent that effective isolation of the waste from the anhydrite interbeds close to the repository could not be fully assured. Because the anhydrite interbeds were known by that time to be relatively more permeable than the halite-rich horizons of the Salado, recognizing that the DRZ was not likely to heal effectively increased the potential importance of interbeds passing through the DRZ with respect to fluid flow in the Salado.

Although panel closures were designed to mitigate operational concerns and that remains their primary purpose, once it was discovered that liquid could be present in the repository it was recognized that panel closures could affect fluid flow there. At first, it was assumed that panel closures would be impermeable and would isolate panels from each other. With recognition that DRZ healing could not be counted on to isolate interbeds from the repository and that fluids might flow around panel closures, for a while the panel closures were essentially assumed not to exist for evaluations of long-term performance. This treatment was unrealistic, however, and the

more reasonable idea that panel closures should be modeled with properties similar to those assigned to the imperfectly healed DRZ gradually emerged.

The conceptual design of shaft seals also changed considerably during the 1980s. The long-term ability of the shaft seals to isolate the repository from overlying units had been credited to a salt component to be emplaced through much of the Salado. The salt-based component would consolidate under the pressure of salt creep and, over a period of a hundred to several hundred years, would develop properties similar to that of intact salt. However, experience with shafts and shaft liners indicated that control of brine flow to the shafts from upper units was of concern. The early concepts of shaft construction, which used a concrete/concrete-grout plug to protect the salt component, were not thought to be robust enough to control such downward brine flow and possibly in the long term to be susceptible to damage by the flow. This concern led to a design and testing program to develop the present shaft concept, which is based on the principle that multiple components and multiple materials provide redundant and demonstrable protection of long-term components from downward brine flow, which supports a high level of confidence in the expected behavior of shaft seals.

Test programs in the upper aquifers have gone on continuously since site selection. As the program matured, the pre-eminent importance of the Culebra Dolomite as a lateral pathway for transport was recognized. The Rustler/Salado contact was demonstrated to be unimportant, and the Magenta Dolomite Member was demonstrated to have generally lower conductivity than the Culebra and not to have hydraulically significant fractures that could channelize flow. Although the Rustler Fm. was characterized to some extent throughout its thickness, in the 1980s the focus came to be on the Culebra. Transport in the Culebra was demonstrated to be controlled by the variation in hydraulic conductivity and by interactions between flow in fractures and flow in matrix. Increasingly complex tests were conducted to characterize the Culebra, including multi-well tracer tests and regional pump tests, culminating in the recent seven-well tracer test conducted at H-19. Increasingly complex modeling techniques were used to represent the characterized variability and residual uncertainty in the hydraulic conductivity of the Culebra, assisted by review and advice from the Geostatistics Expert Group, a panel convened by the WIPP project. Effective chemical and physical retardation was no longer assumed but became the subject of study, and by the time of performance assessments in the early 1990s several alternative conceptual models had been advanced and were implemented; one of these has since been identified as superior to the others.

Ground water has been occasionally encountered in the Dewey Lake Red Beds; because it is not encountered everywhere it had long been assumed that ground water there is in discontinuous lenses, and that regional flow does not occur. Because of this belief, and because of the frustration of trying to characterize ground water in a unit in which ground water is not always encountered, characterizing ground water in the Dewey Lake was a low priority for the WIPP Project. When performance assessments in 1994 showed that long-term releases to the Dewey Lake are unlikely because the Culebra captures all fluids moving upward through the Rustler in a borehole, further characterization of the Dewey Lake was perceived as unimportant. Recently, Project has recognized that there may be a continuous water table in the Dewey Lake, but it is only observed in areas where permeabilities are relatively higher than average. Nevertheless, if

releases into the Dewey Lake occur, they will be of little consequence, because, as a red bed, the Dewey Lake has a uniformly distributed and large sorption capacity.

Geophysical techniques were eventually used to help resolve whether brine reservoirs like that encountered at WIPP-12 might exist in the Castile under the waste panels. These techniques indicated in the late 1980s that brine reservoirs might exist under a portion of the waste disposal area; and the possibility of brine reservoirs has since been important in performance assessments.

The development of probabilistic performance assessments for the WIPP led to a considerable effort to characterize the consequences of combinations of events and processes. One notable development was the identification of the need to model the effects of multiple intrusions into the repository, some of which might penetrate brine reservoirs, and the possible interactions among these intrusions in a partially saturated repository. This led to the identification of the scenarios currently in use.

By the late 1980s, the conceptual model for the repository had changed considerably from that of the late 1970s to mid-1980s. Rather than a fairly simple repository horizon that encapsulated waste rapidly and was thereafter relatively stable, as envisioned until 1985, in 1989 the first SNL preliminary performance assessment recognized that the long-term conditions in the repository depended critically on the interplay between various processes, and the final condition depended closely on the relative rates of these processes. Although uncertainty about many aspects of the disposal system has been substantially reduced through experimental programs and some new release processes have been identified and incorporated since 1989, the overall conceptual model recognized in the late 1980s remains valid today:
- the waste horizon is not effectively isolated from nearby interbeds;
- the repository is partially to fully saturated with liquid;
- gas generation is closely linked to other processes;
- creep closure occurs but does not assure complete consolidation;
- brine inflow from the Salado Fm. is likely;
- high gas pressures in the repository could induce fracturing of Salado interbeds;
- actinide solubilities are important;
- borehole-repository-brine reservoir intersections are possible;
- multiple intrusions allow the possibility of cross-borehole flow;
- the Culebra is the primary upper aquifer, and releases through other units are unlikely;
- Culebra transport is complex, fractures are important, retardation is sensitive.

This list of the major concepts developed in the late 1980s has shaped the thinking about long-term performance, driven the selection of subsequent experimental programs, and determined the types of modeling done in performance assessment from 1989 onward. Since 1989, details have changed, but the overall concept of long-term performance has been stable. The models described in Section 6.4 of the application and further described in this appendix are all based on this overall conceptual understanding of disposal system interactions.

Disposal System
Geometry

1. Model Name

Disposal System Geometry

2. Responsible Contacts

P. Vaughn

3. Model Description and References

The geometry assumed for any model contains important information about the way in which physical processes are thought to act on the system. For the WIPP, the model geometry assumed for the disposal system overall can only be understood in the context of the important processes considered to take place in a particular region during a specific time interval and for a defined purpose. Therefore, the following description of the conceptual model for the disposal system geometry discusses the principal process that is being modeled in conjunction with the geometry of a particular portion of the model. The process most often considered in setting up the domain is fluid flow, because estimates of it are sensitive to the geometry in which it is assumed to occur. Because of the way in which they are conceptualized or mathematically described, many other processes (e.g., creep closure, gas generation, and the formation of dissolved actinides) are sensitive principally to the conditions at a point within the performance assessment domain and not the manner in which points are assumed to be connected through space.

Overall, the conceptual model of the geometry of the disposal system is that the spatial effects of process interactions can be represented in two dimensions. For representing the processes of long-term fluid flow in the Salado Formation, flow between a borehole and overlying units, and flow within the repository (where processes coupled to fluid flow occur, such as creep closure and gas generation), the geometry used is a vertical cross-section through the repository on a north-south axis. The dimension of this geometry in the direction perpendicular to the plane of the cross-section varies to better represent the spatial effects of certain processes, as discussed below.

Three other two-dimensional model geometries are used in performance assessment. For fluid flow and transport modeling in the Culebra Dolomite Member, the geometry is a horizontal two-dimensional plane. For modeling brine flow from the intruded panel to the borehole during drilling, the geometry is a two-dimensional, horizontal representation of a waste panel. For modeling brine flow that might occur between an E1-type borehole and other boreholes penetrating the repository, the geometry used is a two-dimensional, horizontal representation of the entire repository. These geometries are mentioned here but not discussed in detail because they are components of other conceptual models requiring geometric assumptions.

The two-dimensional geometry developed for the Salado Fm. is based on the assumption that brine and gas flow will converge upon and diverge from the repository horizon. The impact of this conceptual model and its implementation in a two-dimensional grid has been compared to

a model that does not make the limiting assumption of convergent and divergent flow as FEP S-1, for which documentation is attached. The conceptual model for the Salado includes the slight and variable dip of beds in the vicinity of the repository, which might affect fluid flow.

Above and below the repository, it is assumed that any flow between the borehole or shaft (see Section 6.4.3) and surrounding materials will converge or diverge. With respect to flow in units overlying the Salado, the only purpose of this conceptual model is to determine the quantity (flux) of fluid leaving or entering the borehole or shaft. Fluid movement through the units above the Salado is treated in a different conceptual model (see Section 6.4.6).

The important distinctions between spatial properties in the conceptual model for the disposal system are again based primarily on fluid flow. Above the Salado, the formations and members that are identified based on geologic or stratigraphic criteria (the unnamed lower member and Culebra Dolomite, Tamarisk, Magenta Dolomite, and Forty-niner Members of the Rustler Fm., the Dewey Lake Red Beds, and near-surface materials) also have hydraulic significance as hydrostratigraphic units (see Section 2.2), and these distinctions are maintained in the conceptual model. Within the Salado, the three geologic members do not have distinct hydraulic significance, and thus these units are not distinguished in the conceptual model. The Salado is conceptualized as having the properties of impure halite. However, near the repository, the interbeds that intersect the DRZ are considered to be hydraulically important and are included in the conceptual model.

Below the repository, the possible presence of a brine reservoir is considered to be important, so a hydrostratigraphic layer representing the Castile and a possible brine reservoir in it is included.

4. Model Purpose

The purpose of the conceptual model for the disposal system geometry is to provide a geometric framework (i.e., a volume within which the spatial relationships of various features are defined) suitable for modeling the interaction of important processes in the disposal system. The principal processes that depend on geometric assumptions are fluid flow and actinide transport; however, effects of processes occurring in only one area within the disposal system, for example gas generation in the repository, may affect fluid flow to some distance.

5. Principal Parameters and Relationship among Parameters Defined by the Model

There are no varied parameters in this model. The principal parameters are the length, width, and height of individual model grid blocks used to discretize the system; these are constant for all realizations and all scenarios.

Disposal System Geometry. The computational model for Brine and Gas Flow (BRAGFLO) uses a single disposal-system geometry with three different maps of material properties: one for undisturbed conditions; one for the E1 intrusion event, in which a borehole
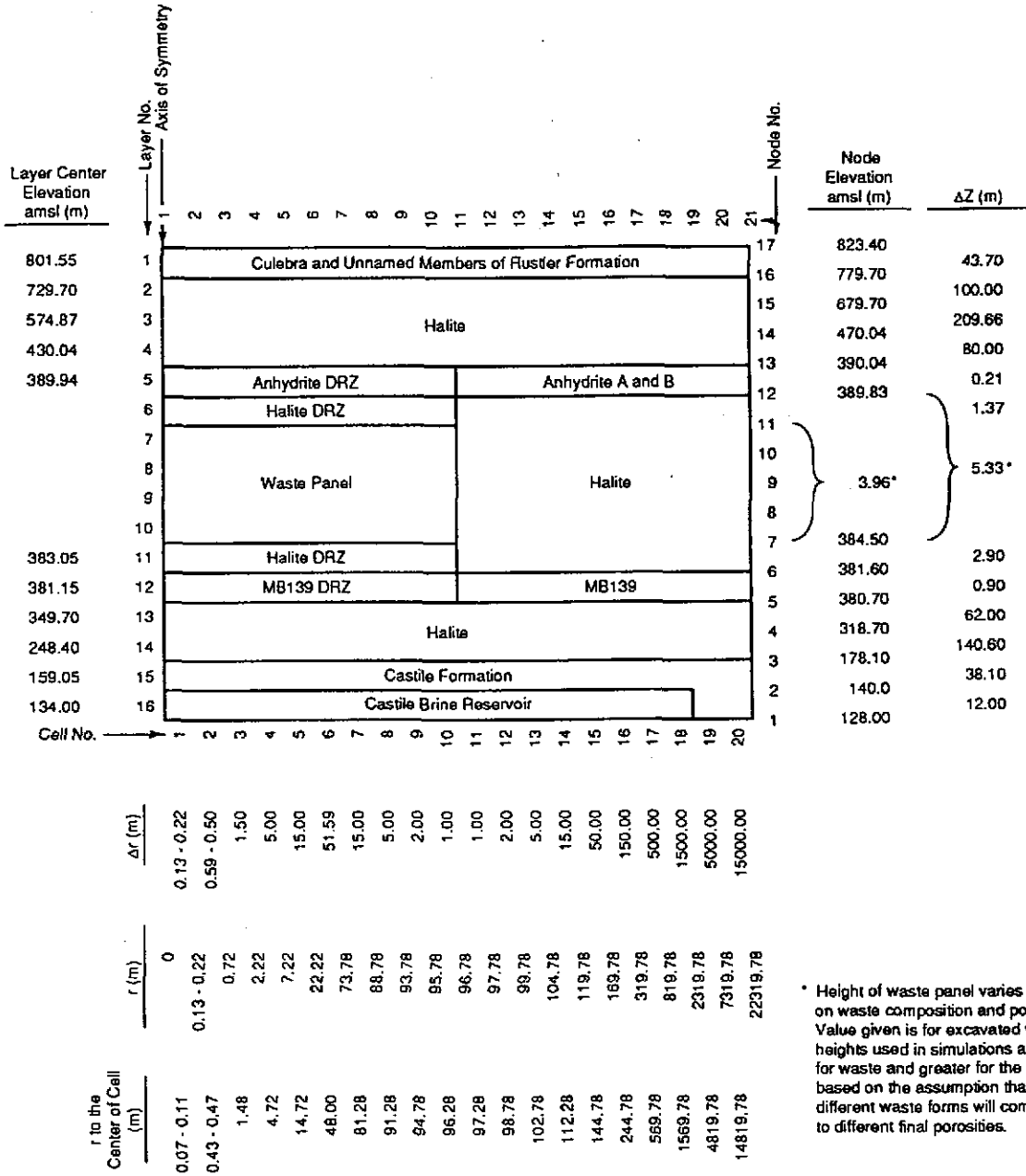
penetrates the repository and Castile brine reservoir; and one for the E2 intrusion event, in which a borehole penetrates the repository but not a Castile brine reservoir.

The disposal-system model has seen numerous changes since the 1991 Preliminary Performance Assessment (WIPP Performance Assessment Department, 1992a, 1992b), when several different geometries were used. For example, the 1992 disturbed performance (E1 and E2) simulations used an equivalent cylindrical panel with the intrusion borehole located at the axis of symmetry (Figure 1; WIPP Performance Assessment Department, 1992a). The use of a single panel implied that the panels were completely isolated from each other. In the 1992 undisturbed simulations two different grid configurations were used (Figures 2 and 3; WIPP Performance Assessment Department, 1992a). Both configurations considered the full repository, including panels, drifts, access shafts, and seals. The second configuration (Figure 3) added the experimental area north of the shaft and consolidated all waste areas into a single region. The four shafts—air intake shaft, salt handling shaft, waste shaft, and exhaust shaft— were combined into a single shaft positioned at the location of the waste handling shaft. Marker Bed 138 was included as an additional potential pathway for flow. None of the 1992 simulations considered the geologic regions above the Culebra; however, uncertainties with regard to long-term shaft seal and borehole performance require that the pathway to the upper regions be considered.
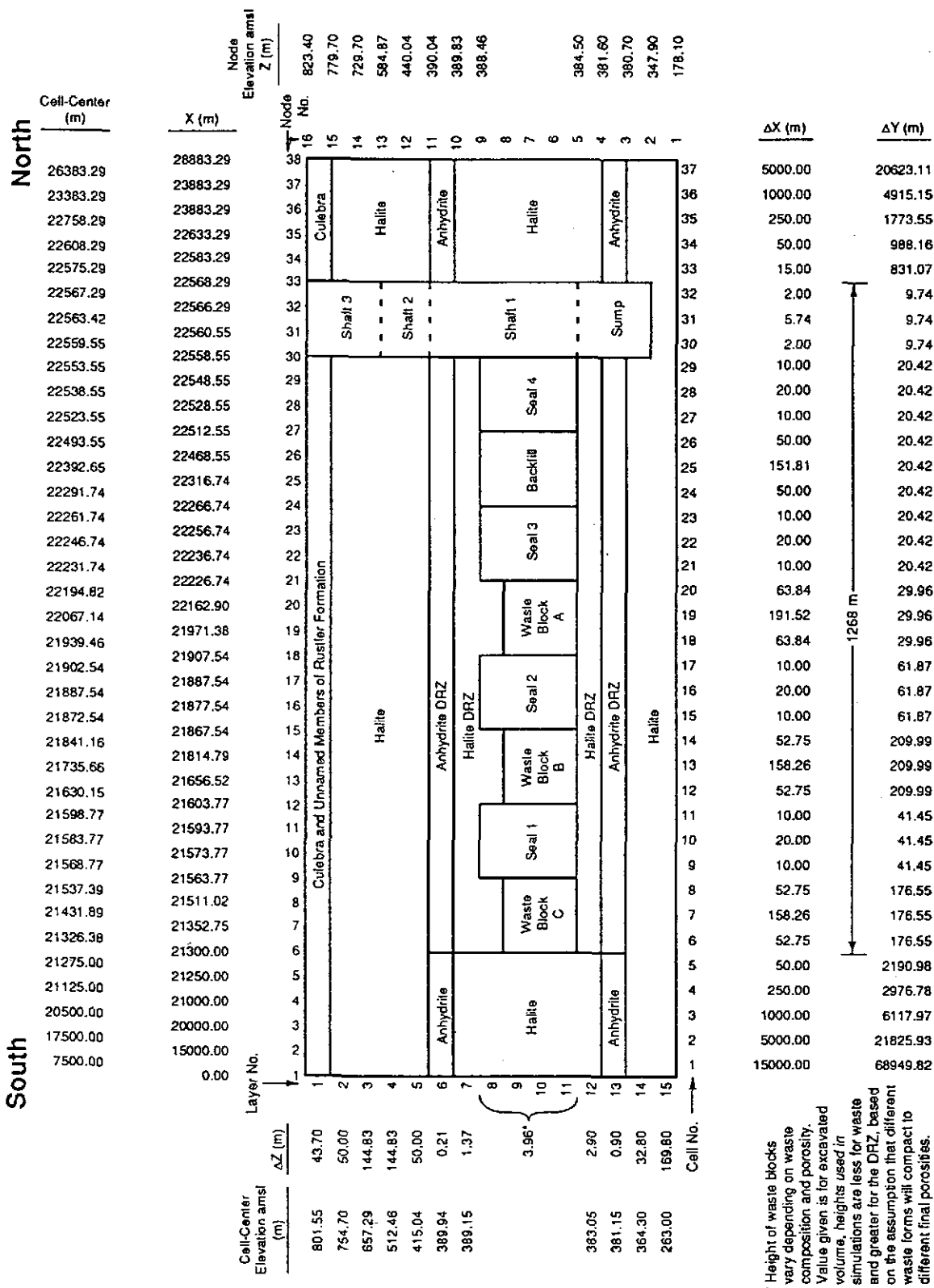
The current disposal system geometry was chosen to allow all simulations, for both disturbed and undisturbed scenarios, to use the same grid description. The repository regions that contain waste have been divided into two sub-regions: a panel region and the remainder of the repository. Separating the panel region allows a more detailed representation of an intrusion borehole penetrating a panel. The effects of inter-panel communication can be examined by varying the permeability of the panel seal. In addition, the Culebra and other geologic units extending to the surface are represented. The various shaft seal components are also included in the modeling. The computational grid used in BRAGFLO is identical for all three scenarios, and the distinction between scenarios is facilitated by introducing material changes at specified time intervals. For example, at the time of an intrusion the material properties corresponding to the borehole grid blocks are changed to those properties consistent with the long term behavior of a borehole and plug system. Additional simulations examining the response immediately following the intrusion are discussed under the heading "direct brine releases."

The simplifying assumption has been made that the three-dimensional physical system can be modeled by considering flow in a two-dimensional plane, oriented north to south, that cuts vertically through the repository and surrounding strata. Effects of flow in the third (out-of-plane) dimension are approximated with a two-dimensional element configuration that simulates convergent or divergent flow to the north and south, centered on the repository, in intact rocks laterally away from the repository. The FEP, S-1, Verification of 2-D WIPP PA Grid Using 3-D Geometry, addresses the appropriateness of this approximation. Based on this FEP, the DOE concluded that although the three-dimensional grid showed flow details that were not accurately represented by the two-dimensional grid, the computed releases to the accessible environment for

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Layer Center Elevation amsl (m) — Layer No. — Axis of Symmetry

Node No. — **Node Elevation amsl (m)** — ΔZ (m)

Node/Cell column numbers: 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21

Layer Center Elevation amsl (m)	Layer No.	Region	Node No.	Node Elevation amsl (m)	ΔZ (m)
			17	823.40	
801.55	1	Culebra and Unnamed Members of Rustler Formation			43.70
729.70	2		16	779.70	100.00
574.87	3	Halite	15	679.70	209.66
430.04	4		14	470.04	80.00
389.94	5	Anhydrite DRZ / Anhydrite A and B	13	390.04	0.21
	6	Halite DRZ	12	389.83	1.37
	7		11		
	8	Waste Panel / Halite	10		5.33*
	9		9	3.96*	
	10		8		
383.05	11	Halite DRZ	7	384.50	2.90
381.15	12	MB139 DRZ / MB139	6	381.60	0.90
349.70	13	Halite	5	380.70	62.00
248.40	14		4	318.70	140.60
159.05	15	Castile Formation	3	178.10	38.10
134.00	16	Castile Brine Reservoir	2	140.0	12.00
			1	128.00	

Cell No. ——→ 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Δr (m): 0.13 - 0.22 | 0.59 - 0.50 | 1.50 | 5.00 | 15.00 | 51.59 | 15.00 | 5.00 | 2.00 | 1.00 | 1.00 | 2.00 | 5.00 | 15.00 | 50.00 | 150.00 | 500.00 | 1500.00 | 5000.00 | 15000.00

r (m): 0 | 0.13 - 0.22 | 0.72 | 2.22 | 7.22 | 22.22 | 73.78 | 88.78 | 93.78 | 95.78 | 96.78 | 97.78 | 99.78 | 104.78 | 119.78 | 169.78 | 319.78 | 819.78 | 2319.78 | 7319.78 | 22319.78

r to the Center of Cell (m): 0.07 - 0.11 | 0.43 - 0.47 | 1.48 | 4.72 | 14.72 | 48.00 | 81.28 | 91.28 | 94.78 | 96.28 | 97.28 | 98.78 | 102.78 | 112.28 | 144.78 | 244.78 | 569.78 | 1569.78 | 4819.78 | 14819.78

* Height of waste panel varies depending on waste composition and porosity. Value given is for excavated volume, heights used in simulations are less for waste and greater for the DRZ, based on the assumption that different waste forms will compact to different final porosities.

Figure 1. Geometry of the cylindrical equivalent panel model used in the 1992 performance assessment (WIPP Performance Assessment Department, 1992a).

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North / **South**

Cell-Center (m)	X (m)	Node No.
26383.29	28883.29	38
23383.29	23883.29	37
22758.29	23883.29	36
22608.29	22633.29	35
22575.29	22583.29	34
22567.29	22568.29	33
22563.42	22566.29	32
22559.55	22560.55	31
22553.55	22558.55	30
22538.55	22548.55	29
22523.55	22528.55	28
22493.55	22512.55	27
22392.65	22468.55	26
22291.74	22316.74	25
22261.74	22266.74	24
22246.74	22256.74	23
22231.74	22236.74	22
22194.82	22226.74	21
22067.14	22162.90	20
21939.46	21971.38	19
21902.54	21907.54	18
21887.54	21887.54	17
21872.54	21877.54	16
21841.16	21867.54	15
21735.66	21814.79	14
21630.15	21656.52	13
21598.77	21603.77	12
21583.77	21593.77	11
21568.77	21573.77	10
21537.39	21563.77	9
21431.89	21511.02	8
21326.38	21352.75	7
21275.00	21300.00	6
21125.00	21250.00	5
20500.00	21000.00	4
17500.00	20000.00	3
7500.00	15000.00	2
	0.00	1

Node Elevation amsl Z (m) (Node No.):
823.40 (16), 779.70 (15), 729.70 (14), 584.87 (13), 440.04 (12), 390.04 (11), 389.83 (10), 388.46 (9), 384.50 (5), 381.60 (4), 380.70 (3), 347.90 (2), 178.10 (1)

Cell No.	ΔX (m)	ΔY (m)
37	5000.00	20623.11
36	1000.00	4915.15
35	250.00	1773.55
34	50.00	988.16
33	15.00	831.07
32	2.00	9.74
31	5.74	9.74
30	2.00	9.74
29	10.00	20.42
28	20.00	20.42
27	10.00	20.42
26	50.00	20.42
25	151.81	20.42
24	50.00	20.42
23	10.00	20.42
22	20.00	20.42
21	10.00	20.42
20	63.84	29.96
19	191.52	29.96
18	63.84	29.96
17	10.00	61.87
16	20.00	61.87
15	10.00	61.87
14	52.75	209.99
13	158.26	209.99
12	52.75	209.99
11	10.00	41.45
10	20.00	41.45
9	10.00	41.45
8	52.75	176.55
7	158.26	176.55
6	52.75	176.55
5	50.00	2190.98
4	250.00	2976.78
3	1000.00	6117.97
2	5000.00	21825.93
1	15000.00	68949.82

1268 m

Region labels: Culebra; Halite; Anhydrite; Halite; Anhydrite. Shaft 3; Shaft 2; Shaft 1; Sump. Culebra and Unnamed Members of Rustler Formation. Anhydrite DRZ; Halite DRZ; Halite DRZ; Anhydrite DRZ; Halite. Seal 4; Backfill; Seal 3; Waste Block A; Seal 2; Waste Block B; Seal 1; Waste Block C. Anhydrite; Halite; Anhydrite.

Layer No.	ΔZ (m)	Cell-Center Elevation amsl (m)
1	43.70	801.55
2	50.00	754.70
3	144.83	657.29
4	144.83	512.46
5	50.00	415.04
6	0.21	389.94
7	1.37	389.15
8–11	3.96*	
12	2.90	363.05
13	0.90	381.15
14	32.80	364.30
15	169.80	263.00

* Height of waste blocks vary depending on waste composition and porosity. Value given is for excavated volume, heights used in simulations are less for waste and greater for the DRZ, based on the assumption that different waste forms will compact to different final porosities.

Figure 2. Geometry of the two-dimensional vertical cross-section model of the full repository used in the 1992 performance assessment (WIPP Performance Assessment Department, 1992a).
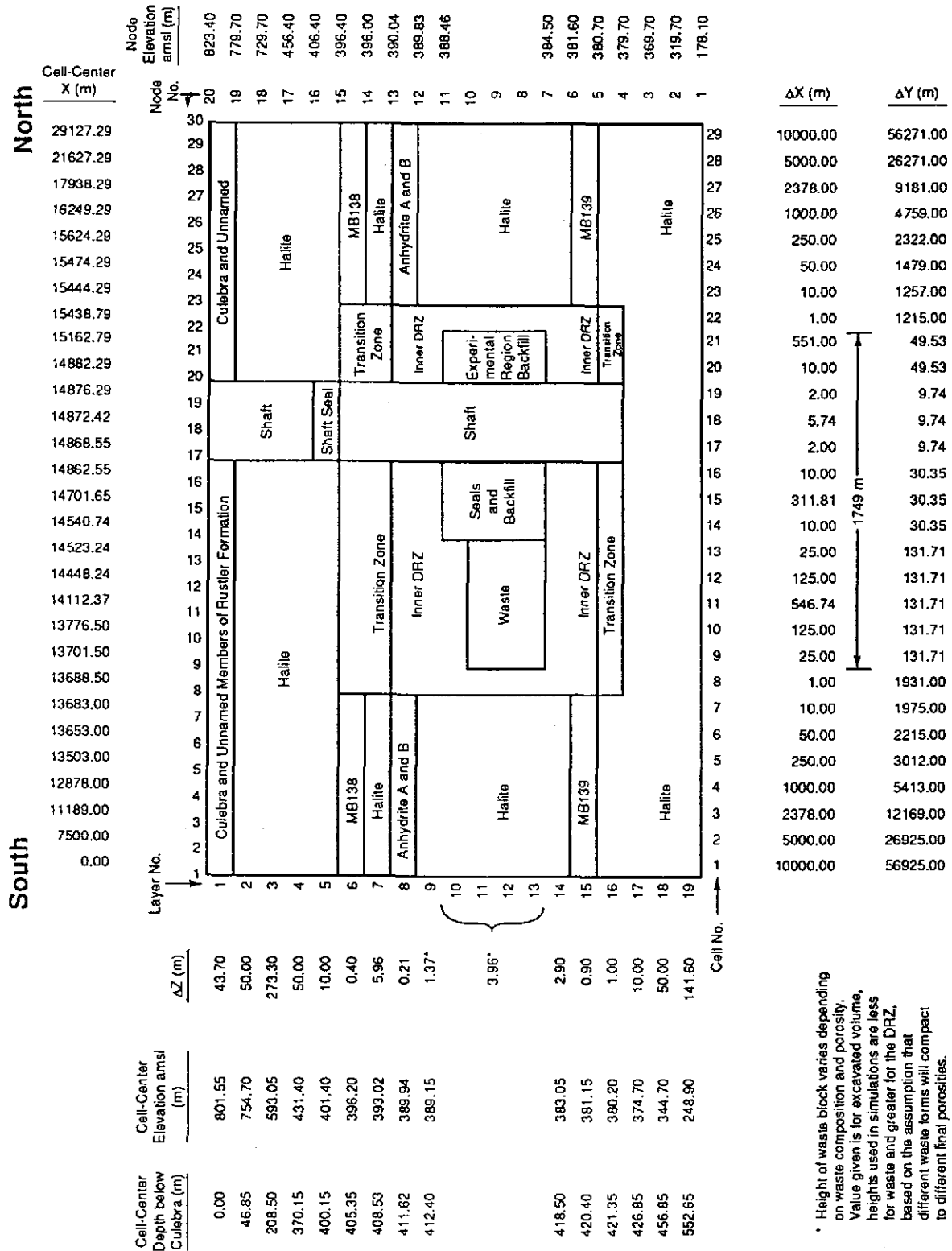
Figure 3. Geometry of the two-dimensional vertical cross-section model used in the 1992 performance assessment (WIPP Performance Assessment Department, 1992a).

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both grids were nearly equivalent. This indicates that, based on the performance measures and the overall uncertainty, the current model being used for WIPP Performance Assessment is sufficient for estimates of calculated releases. Calculations using the two-dimensional grid are more computationally efficient, which is necessary for the large number of vectors.

Side views of the vertical cross section and two material maps are presented in Section 6.4.2. In these figures, the boundaries of grid blocks discretized in the model are shown with dashed lines; each grid block is associated with material properties representing an important feature of the disposal system. These associations between grid blocks and material properties are shown by color and number in the figures. The two figures differ in that the material property map used for E1 intrusion events includes a material region representing the borehole (Region 1) that is not present in the undisturbed case. The borehole region vertically transects other material regions and connects the single panel (Region 23) with the Castile brine reservoir (Region 30), marker beds, overlying units, and the surface. The E2 intrusion material regions are similar to those of E1, except that the modeled borehole region does not extend below the repository and therefore does not contact a brine reservoir.

The figures show the relationship among material regions in the model and how connections are made within the finite-difference scheme. However, by illustrating equidimensional grid blocks, the volumetric relationship between grid blocks is greatly distorted. To show the volumetric relationship among nodal blocks and between the repository and host formations, a scaled, side view of the vertical cross section used in BRAGFLO is also shown and discussed in Section 6.4.2.

Beds in the Salado dip generally to the south in the immediate vicinity of the repository. The DOE approximates the variable dip in the Salado by incorporating a 1-degree dip to the south in the BRAGFLO computational mesh, although it is not illustrated in Section 6.4.2. Webb and Larson (1996) discussed the effect of stratigraphic dip on brine and gas flow.

The BRAGFLO definition of hydrostratigraphic units follows formation and member divisions. Inside the Salado Fm., however, the hydrostratigraphy has been further subdivided based on the observed differences in permeability between anhydrite-rich interbeds and halite-rich intervals. This subdivision has been made only at altitudes near the repository horizon because only in this region are such distinctions important. Frear and Webb (1996) examined the impact of stratigraphic layers on brine and gas flow.

The flow fields generated by the BRAGFLO simulations are used by the transport code NUTS to determine the transport of nuclides to the accessible environment. BRAGFLO results are communicated to NUTS using a binary file. Several other models use BRAGFLO simulation results, e.g., the direct brine release model and the CUTTINGS model.

References:

Christian-Frear, T.L., and S.W. Webb. 1996. *Effect of Explicit Representation of Detailed Stratigraphy on Brine and Gas Flow at the Waste isolation Pilot Plant.* SAND94-3173. Albuquerque, NM: Sandia National Laboratories

Webb, S.W., and K.W. Larson. 1996. *The Effect of Stratigraphic Dip on Brine and Gas Migration at the Waste Isolation Pilot Plant.* SAND94-0932. Albuquerque, NM: Sandia National Laboratories

WIPP Performance Assessment Department. 1992a. *Long-Term Gas and Brine Migration at the Waste Isolation Pilot Plant: Preliminary Sensitivity Analyses for Post-Closure 40 CFR 268 (RCRA), May 1992.* SAND92-1933. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992b. *Preliminary Performance Assessment for the Waste Isolation Pilot Plan, December 1992- Volume 5: Uncertainty and Sensitivity Analyses of Gas and Brine Migration for Undisturbed Performance.* SAND92-0700. Albuquerque, NM: Sandia National Laboratories.

Culebra Geometry

1. Model Name

Conceptual model for the geometry used in two-dimensional modeling of ground-water flow in the Culebra Dolomite Member of the Rustler Formation.

2. Responsible Contacts

J. Ramsey and M. LaVenue (Intera)

3. Model Description and References

The SECOFL2D code uses two two-dimensional horizontal grids to simulate ground-water flow. A regional grid approximately 22 by 30 km is used to determine the flow fields in the WIPP region resulting from hydraulic head distributions controlled by distant topographic and hydrologic features (i.e., boundary conditions) and the regional distribution of transmissivity in the Culebra. Because this grid is used to define boundary conditions for the flow and transport calculations, it is discussed in detail in Section 6.4.10.2, together with the specification of initial and boundary conditions. A local grid 7 by 7 km with finer discretization is used in both SECOFL2D and SECOTP2D in the region of interest—in the controlled area and its immediate vicinity—to provide additional resolution for flow and transport to the accessible environment. Boundary heads and fluxes for the local grid are obtained by interpolation from the regional flow field.

The grid for the local domain contains 75 columns and 65 rows, resulting in 4875 grid blocks. Boundaries of the local domain were chosen to capture important flow paths and facilitate the computation of integrated release to the accessible environment. Because ground-water flow from the region above the panels is to the south and is most rapid to the west, the local domain extends slightly beyond the southern and western boundaries of the controlled area. A small strip in the northern portion of the controlled area has been omitted from the local domain to allow increased resolution in the area of interest to the south.

See also:

The geometry used in SECOFL2D and SECOTP2D simulations are described in Section 6.4.2.2.

Initial and boundary conditions for SECOFL2D used in the Compliance Certification Application are described in Section 6.4.10.2 and Appendix TFIELD.

4. Model Purpose

The geometry used in the SECOFL2D and SECOTP2D Culebra model are chosen to provide a reasonable and realistic basis for two-dimensional simulations of ground-water flow and radionuclide transport through the Culebra.

5. Principal Parameters and Relationships among Parameters Defined by the Model

Dimensions of the model domain and grid blocks are discussed in Section 3 above. Parameters used in the Culebra model are discussed in sections related to flow and transport modeling.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

As discussed below in Section 8, past analyses have considered different domains for two-dimensional flow in the Culebra. The current approach, using a local domain nested within a regional domain, was developed in 1991 to reduce the sensitivity of model results to the dimensions of the domain.

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

Since the Final Environmental Impact Statement (FEIS) in 1980, the conceptual model used to describe flow and transport within the Culebra has changed significantly. In the FEIS, the Culebra and the Magenta were combined and modeled as one layer and referred to as the "Rustler aquifers." A uniform transmissivity field was assumed across the model domain except in Nash Draw. Regional flow was assumed to be toward the southwest, discharging at Malaga Bend on the Pecos River. The formation fluid density within the Culebra was treated being equal to fresh water, and therefore the model was unable to consider possible effects of brine density on ground-water flow.

In 1987, a new model (Haug et al., 1987) used a more developed conceptual model of the Culebra flow domain. The objective of this study was to calibrate a flow model to the H-3 pumping test and the effects from the excavation of the shafts. Numerous new boreholes had been installed and tested since the 1980 study, and test results were considered in the model. The boundaries of the model were not much larger than the extent of the WIPP-site boundary. Brine densities were also used as a calibration target. The brine densities were assigned at the boundaries and subsequently modified to match the observed fluid densities. Vertical recharge was included in this model in an attempt to calibrate the brine densities. The transmissivity field was estimated by kriging and modified by the addition of pilot points, which were located by trial and error. Single- and dual-porosity effects on the flow field were investigated. It was determined that at the regional scale, the use of a dual-porosity vs. single-porosity conceptual model had very little effect on the flow field.

A modeling study conducted to support the Draft Supplemental Environmental Impact Statement (DSEIS) (LaVenue et al., 1988, 1990) only slightly modified the conceptual model used by Haug et al. (1987). The difference in the conceptual model was the assumption that brine density was variable but fixed over the time scale of the model (i.e., ten years). It was

assumed that the brine concentrations could be taken to be at quasi-steady state over this period of time. The boundaries of the 1988 study were much larger than the 1987 study, extending ~30 km north and south and 20 km east and west. The model grid was centered on the WIPP site. The boundaries were selected to maximize the use of regional freshwater heads and to minimize the boundary effects during transient simulation of the H-3, WIPP-13, and H-11 pumping tests. Vertical recharge was not included. Fixed heads were assigned around all four boundaries based on regional head values. Transmissivities were estimated by kriging and ranged over seven orders of magnitude in this study. Pilot points were added to modify the transmissivity field during steady-state and transient calibration. Pilot point locations were selected using an adjoint sensitivity analysis technique.

Multiple transmissivity fields were generated and were subsequently calibrated to the same steady-state and transient events used in the 1988 model. The main differences in the 1988 and 1992 models were the model boundary locations, boundary conditions, and the geostatistical approach used to develop and modify the transmissivity field. The 1992 model boundaries were rotated 38 degrees east to align with the axis of Nash Draw. This permitted the specification of a no-flow boundary along a portion of the western boundary coinciding with the Nash Draw axis. In addition, the northeastern corner of the model was also considered as a no-flow boundary because of the low transmissivities in the area and the lack of any nearby regional heads to provide boundary head estimates. Transmissivities were simulated by conditional simulation. Pilot points were automatically located and assigned transmissivity values through an optimization routine during steady-state and transient state calibration.

References:

Haug, A., V.A. Kelley, A.M. LaVenue, and J.F. Pickens. 1987. *Modeling of Ground-Water Flow in the Culebra Dolomite at the Waste Isolation Pilot Plant (WIPP) Site: Interim Report.* SAND86-7167. Albuquerque, NM: Sandia National Laboratories.

LaVenue, A.M., A. Haug, and V.A. Kelley. 1988. *Numerical Simulation of Ground-Water Flow in the Culebra Dolomite at the Waste Isolation Pilot Plant (WIPP) Site. Second Interim Report.* SAND88-7002. Albuquerque, NM: Sandia National Laboratories.

LaVenue, A.M., T.L. Cauffman, and J.F. Pickens. 1990. *Ground-Water Flow Modeling of the Culebra Dolomite. Volume 1: Model Calibration.* SAND89-7068/1. Albuquerque, NM: Sandia National Laboratories.

9. Information Supporting Model Choice and Confirmation

See Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See Section 8.

The Repository

1. Model Name

The Repository

2. Responsible Contact

P. Vaughn

3. Model Description and References

This conceptual model represents the geometry of the repository used for performance assessment. As with the geometry of the disposal system discussed in Section 6.4.2.1, the principal process considered in setting up the repository geometry is fluid flow. Several features of the repository considered to be important in fluid flow are included in the conceptual model. The first is the overall dimension of the repository along the north-south trend of the cross section, as well as the major divisions within the repository (waste disposal panels, operations region, and experimental region). The second is the volume of a single panel, because fluid flow to a borehole penetrating the repository can potentially access only the volume in a waste panel directly and other regions of the repository only by flow through or around a panel closure. The third is the physical dimensions of panel closures separating the single panel and the other major divisions of the repository. In determining the appropriate way to represent these features, the important concepts applied are to preserve dimensions along the axis of the model, interface areas, and volumes excavated.

Notably absent from the conceptual model for the long-term performance of the repository are pillars and individual drifts and rooms. These are excluded from the model for simplicity, and it is assumed that they have either negligible impact on fluid flow processes or, alternatively, that including them in the conceptual model would be beneficial to long-term performance because their presence could make flow paths more tortuous and decrease fluxes.

Nine of the equivalent panels in the waste disposal area are not explicitly modeled, but instead are lumped together in one region for simplicity. In this region, panel closures and pillars are excluded. It is assumed that including these panel closures would be beneficial to performance because they have properties that are less transmissive than waste areas, and they would make flow paths more tortuous.

4. Model Purpose

The purpose of this model is to provide a reasonable representation of the geometry of the WIPP repository with respect to the interactions between important processes that occur there.

5. Principal Parameters and Relationship among Parameters

There are no varied parameters in this model. The principal parameters are the length, width, and height of individual model grid blocks used to discretize the repository; these are constant for all realizations and all scenarios. See also Section 6.4.3.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The BRAGFLO model of the WIPP disposal system is a two-dimensional array of three-dimensional grid blocks. Each grid block has a finite length, width, height, volume, and surface area for its boundaries with neighboring grid blocks. The BRAGFLO two-dimensional grid is similar to any other two-dimensional grid used to treat flows, except that the grid-block dimension in the direction perpendicular to the grid (z-direction) varies from block to block as a function of the lateral direction (x-direction). This allows the BRAGFLO grid to treat important geometric aspects of the WIPP disposal system, such as the very small intrusion borehole, the moderate-size shaft, and the large land withdrawal region.

In two-dimensional fluid-flow codes, a grid block's length, volume, and cross-sectional area of faces connected to other grid blocks are important model features. For each region of the repository depicted, the BRAGFLO model geometry preserves the true excavated volume. Lateral dimensions have been determined to preserve volume and retain important cross-sectional areas and distances between defined regions. These simplifications are conservative with respect to fluid contact with waste, which is a critical factor in determining the quantity of actinides mobilized in the aqueous phase. The simplifications are conservative for two reasons: all pillars have been removed from panels, resulting in homogeneous waste regions through which fluid can flow directly; and the panels in the rest of the repository have neither pillars nor closures, resulting in a very large region of homogeneous waste that is assigned high permeabilities within the reasonable range of possible permeabilities.

7. FEPs Associated with Model Development

DR2, Wicking Around Waste Drums
GG1, Radiolysis of Brine
GG2, Gas Generation (Reaction Path Model)
DR3, Closure of Unfilled North End
DR6, Puddling
DR7, Permeability a Function of Porosity
DR8, Threshold Displacement Pressure a Function of Permeability
DR9, Anhydrite Threshold Displacement Pressure a Function of Permeability
DR4, Circulation of Fluid in Repository up Borehole to Surface After Intrusion
DR5, Recirculation of Castile Brine Through Waste and to Surface (Single Borehole)

8. History of Model Development and Alternatives Considered and Rejected

Several early models of repository fluid-flow behavior (models of radionuclide migration pathways, gas flow from the disposal area to the shaft, Salado brine flow through panel to borehole, effects of anhydrite layers on Salado brine flow through a panel, and flow from a brine pocket through a disposal room) are summarized in a 1990 report (Rechard et al., 1990).

In the Preliminary Performance Assessment of 1992, all waste was lumped into a single region (WIPP PA Dept. 1993). Because human intrusion boreholes must be treated in detail for

the 1996 CCA (Marietta et al., 1989), it was necessary to model a single waste panel with a borehole surrounded by two-dimensional radial-flaring gridblocks. The remainder of the waste is modeled as the rest of the repository and is separated from the waste panel by a panel closure.

References:

Rechard, R.P., W. Beyeler, R.D. McCurley, D.K. Rudeen, J.E. Bean, and J.D. Schreiber. 1990. *Parameter Sensitivity Studies of Selected Components of the Waste Isolation Pilot Plant Repository/Shaft System.* SAND89-2030. Chapter 5, Summary and Conclusions, pp. 153 - 160.

WIPP Performance Assessment Department. 1993. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992, Volume 4: Uncertainty and Sensitivity Analyses for 40 CFR 191, Subpart B,* Section 4.1, Model Geometry, pp. 4-1, 4-3, SAND92-0700/4.

Marietta, M.G., S.G. Bertram-Howery, D. R. (Rip) Anderson, K.F. Brinster, R.V. Guzowski, H. Iuzzolino, R.P. Rechard. 1989. *Performance Assessment Methodology Demonstration: Methodology Development for Evaluating Compliance with EPA 40 CFR 191, Subpart B, for the Waste Isolation Pilot Plant.* SAND89-2027. pp. III-4 through III-16, and pp. IV-2 through IV-49.

9. Information Supporting Model Choice and Confirmation

The single panel that is represented individually (Region 23) is discretized to simulate radial flow to and from the borehole that intersects it. The true distance from the south end of the waste disposal region to the waste handling shaft is preserved in the model as the distance from the south end of the modeled panel to the modeled single shaft. In BRAGFLO, the single panel region is the southernmost portion of the repository. It occupies this position because separate modeling indicated that slightly larger releases may result from a panel in this position than from alternative placements (Webb and Larson, 1996).

The panel closure between the panel and the rest of the repository has a cross-sectional area equal to the cross-sectional area of the drifts between panels. The length and total volume of modeled panel closures is consistent with their design. The panel closure between the rest of the repository and the operations region has a cross-sectional area equal to the cross-sectional area of the drifts between the north end of the waste disposal region and the operations region. Because there are two sets of closures between the waste disposal region and the shafts in the operations region, the panel closures between the rest of the repository and the operations region have a length and volume consistent with two sets of panel closures.

See also the corresponding information for the individual models relevant to the repository region (Creep Closure, Repository Fluid Flow, Gas Generation, Chemical Conditions in the Repository, Dissolved Actinide Source Term, and Colloidal Actinide Source Term).

References:

Webb, S.W. and K.W. Larson. 1996. *The Effect of Stratigraphic Dip on Brine Inflow and Gas Migration at the Waste Isolation Pilot Plant*. SAND94-0932.

10. Validity and Completeness Interface/Integration with PA and Computational Models

A number of submodels have been defined within the repository region. The submodels that have been defined for repository processes are Creep Closure (Section 6.4.3.1), Repository Fluid Flow (Section 6.4.3.2), Gas Generation (Section 6.4.3.3), Chemical Conditions in the Repository (Section 6.4.3.4), Dissolved Actinide Source Term (Section 6.4.3.5), and Colloidal Actinide Source Term (Section 6.4.3.6).

Creep Closure

1. Model Name

Creep Closure

2. Responsible Contact

Barry Butcher

3. Model Description and References

Salt creep occurs naturally in the Salado halite in response to deviatoric stress. This process was recognized as beneficial in the original siting of the repository and is considered important in the overall conceptual model for long-term performance. Inward creep of rock and the repository response, generally called creep closure, embodies several important concepts. Creep closure of excavated regions begins immediately because of excavation-induced deviatoric stress. If the rooms were empty, closure would continue until the void volume created by the excavation was eliminated as the surrounding formation returns to a uniform stress state. This will occur in the operations region and experimental region. In the waste disposal region, waste consolidation will continue until loading in the surrounding rock is uniform, at which point salt creep ceases. The amount of waste consolidation that occurs and the time it takes to consolidate are governed by properties of the waste (waste strength), properties of the surrounding rock, the dimensions and location of the room, and the quantities of fluids present in the room.

Fluids that could affect closure are brine entering the repository from the Salado or an intrusion borehole, air present in the repository when it is sealed, and gas produced by reactions occurring during waste degradation. Closure and consolidation can be slowed by fluid pressure in the repository. This can be quantified according to the principle of effective stress:

$$\sigma_T = \sigma_e + p \ ,$$

where σ_T is the stress caused by the weight of the overlying rock and brine (an essentially constant value), p is the pressure of the repository pore fluid, and σ_e is the stress applied to the waste skeleton or matrix. In this formulation, the waste is considered to be a skeleton structure immersed in pore fluids. As the pore pressure increases, an increasing amount of overburden stress is supported by pore fluid pressure, and less overburden stress is supported by the strength of the waste matrix. Because of waste strength, waste consolidation can cease even if pore fluid pressures do not reach lithostatic pressure. If gas and brine quantities in the repository stabilize, creep closure will act to establish a constant pressure and pore volume.

In summary, creep closure of waste disposal areas will cause their volume to decrease as the Salado deforms to consolidate and encapsulate the waste, changing waste porosity and permeability. Waste strength and fluid pressure will resist creep closure.

4. Model Purpose

This model represents the effects of deformation of halite in the Salado Fm. on the volume of void space in the repository through time.

5. Principal Parameters and Relationship among Parameters Defined by the Model

The principal parameters defined by the conceptual model for creep closure depend on the mathematical representation chosen to model these concepts. The precise definition of the mathematical equations and important parameters used to model the creep closure behavior of the repository will be documented in Appendix PORSURF, which describes the SANTOS code, with which they are implemented. Generally speaking, the important parameters in models of creep closure are those used to describe the behavior or strength of materials when they are subjected to various stresses. Within the repository, the extent of creep closure depends on interactions not only with parameters defined by the creep closure model *per se*, but also on the outcomes or feedback with processes simulated with other models. The extent of creep closure is closely linked to the models that determine the fluid saturation and pressure in the repository (Salado flow, borehole flow), and to the gas generation model, which influences repository pressure. The creep closure model feeds back on the fluid flow models by influencing pressure and liquid saturation in the repository as creep closure changes void volume.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The principal uncertainties in creep closure are several. The first source is attributed to the need for simplification and inability to characterize the waste in order to develop a mathematical model of its response. Testing radioactive materials has always been considered unfeasible, and waste surrogate materials had to be defined that were sufficiently uniform and well-defined to permit recovery of mechanical and physical property information from the literature or meaningful measurements in the laboratory. Formulation of realistic mathematical response was challenging because even the surrogate materials were complex.

Two complicating factors were (1) the continual change in perception of the types and amounts of waste to be stored in WIPP because of updated inventory projections, and (2) changes in the properties of the waste after emplacement in the repository by biodegradation and corrosion. For example, vitrified waste is expected to respond mechanically to closure much differently than unprocessed waste. Uncertainty about emplaced waste arises from the uncertainty about the physical nature of reaction products, what intermediate states of biodegradation are like, and whether the corrosion product for iron behaves as a rigid granular material or is more like a plastic material. Any change in the waste therefore has the potential for altering certain details of the creep closure conceptual model, although the basic concept of waste entombment by salt remains the same. Resolution of these details is unlikely; however, in the sense that rapid creep closure is considered more desirable than slow closure, the model used for the CCA is considered conservative. It is unlikely that closure for future waste iterations will ever take longer than closure for unprocessed, undegraded waste with no backfill. (This discussion applies only to a backfill, such as crushed salt, that might be emplaced for mechanical

purposes, such as accelerating waste encapsulation. It does not apply to backfill emplaced to affect repository chemistry.)

If backfill is emplaced, its deformation with time is another major uncertainty in defining the effects of creep closure on the waste. If backfill is used, one of the most important considerations is whether it is emplaced in the empty space between the waste containers, since this consideration can influence how consolidation of the waste is modeled.

The second type of parameter having great impact on the processes depicted in the conceptual model is related to simplification of the geometric representation of the disposal room in order to model it mathematically. At this time, technical feasibility limits most calculations to a single disposal room configuration. Waste contained within the room is represented in terms of its response averaged over the volume of the room. Panel-wide and repository-wide three-dimensional calculations have not been performed, nor are they considered essential.

Even at the room scale, random emplacement of the various types of waste is assumed. The room is assumed to contain the maximum amount of waste in a perfectly close-packed configuration, although this is probably impossible to achieve in practice.

The uncertainties discussed above may be unimportant, however, because the exact state of the contents within the disposal room has never been identified by performance assessment analyses as a critical parameter. One explanation for this lack of sensitivity is that the waste appears to be so permeable that details associated with the waste state are not critical. For example, fluid flow through the waste can be considered to be instantaneous in comparison with flow through the other elements in the flow paths, and insufficient void volume exists within the waste to contain all the gas that might be potentially produced. Therefore, while the details of application of the creep conceptual model may introduce a degree of uncertainty, this uncertainty is considered negligible in comparison with other processes controlling release.

7. FEPs Associated with Model Development

DR-12, Dynamic Closure (Coupling with Flow)
DR-3, Dynamic Closure of the North End and Hallways

8. History of Model Development and Alternatives Considered and Rejected

Development of the creep closure conceptual model for the CCA is the result of a large number of investigations over the past ten years. Evolution of this development is shown pictorially in Section 2.3 of Butcher et al. (1994) and discussed in more detail in Chapter 3 of the report. Very basic considerations at the beginning of the development period were whether creep closure had to be modeled three-dimensionally or whether a two-dimensional representation was adequate. Definition of how much of the global stress field surrounding the repository had to be included in the model and the importance of three-dimensional stress effects at drift intersections had to be resolved. The conclusion of these studies was that a two-dimensional representation of waste storage on the room scale, as opposed to a panel- or repository-wide scale, would suffice.

Once a room-scale representation was adopted, the question of whether it should be an isolated room or a room in an infinite array of rooms (an array room) was considered. After establishing the difference between closure for the two representations, an array room, closely analogous to the center room in a panel, was selected in preference to an isolated room. At one time a quarter-room symmetry representation of the array room was adopted to reduce computational time. The quarter-room symmetry representation neglected the effects of gravity. More recently all calculations have been with a half-room symmetry, which exactly represents closure response for the array room configuration. Although studies with the more-exact model continued to showed that gravity effects were minimal, the half-room symmetry model continues to be used because the quarter-room symmetry model does not adequately represent the nonsymmetrical feature of an air gap above the waste (or waste and backfill).

The extent of detail for the model representing creep of the surrounding salt was important from the beginning of development because simpler representations are less demanding on computer resources. This part of the development of the conceptual model primarily influences whether transient creep behavior must be included in the creep description. Although early calculations were made with a simplified halite creep model, all recent calculations have been made with the Multimechanism Deformation Model, which includes transient response and has become the standard for WIPP creep analyses.

The model used for the CCA is considered to be conservative because rapid creep closure is considered more desirable than slow closure. It is unlikely that closure for possible future waste iterations will be longer than closure for unprocessed, undegraded waste with no backfill. In keeping with this observation, an enhanced creep controlled by the temperature of localized regions within the repository has never been considered in calculations. Increases in temperature could arise from radioactive decay or release of energy during chemical reactions. Instead creep closure around the disposal room has been assumed to occur in an isothermal environment at a temperature of 300 K. Although the model can handle increases in temperature, their quantification would be difficult. The justification for assuming an isothermal state is that any temperature increase would cause more rapid closure, a situation more desirable from the viewpoint of room performance than the present model. In this sense, therefore, the current model is conservative.

The degree of stratigraphic detail necessary has always been of concern in creep closure calculations because the full stratigraphic detail of the repository surrounds is more than can be routinely included in calculations. Early approximations treated the rock surrounding a disposal room as pure salt, thereby completely neglecting the possible influence of the interbeds and clay seams closest to the repository horizon. This approximation was considered too simplistic, however. After studies of the effects of varying detail in the stratigraphy, a simplified stratigraphy has been adopted to recognize regions of pure halite and impure halite and principal interbeds closest to the repository horizon.

Several alternative models of material response were also investigated during evolution of the model for creep closure. Because the evolution of these models is not really related to conceptual model development, but rather constitute its translation into mathematical models, the

history of their development is not included here. (For further information, see Butcher et al., 1994, Chapter 3.) The effects of gas also fall into this category. Perhaps the only model consequence of gas generation is the assumption that gas can permeate the waste materials, which then respond as a solid skeleton structure surrounded by gas; that is, gas is considered to flow freely through the waste unless brine is present, equalizing local gas pressurization. The computational method most appropriate for representing the conceptual model has been a topic of extensive study. The main concern related to computations is the method of accounting for the influence of fluid flow processes on creep closure, specifically the availability of brine as a reactant in gas generation by iron corrosion.

References:

Butcher, B. M., Webb, S. W., and Berglund, J. W. 1994. "Disposal Room and Cuttings Models - White Paper for Systems Prioritization and Technical Baseline," WIPP Project document.

9. Information Supporting Model Choice and Confirmation

See Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models

Computational data from creep closure calculations, describing creep closure around the waste in terms of porosity or gas pressure as a function of time for various assumed gas generation histories, serve as input to BRAGFLO. Although the scale and geometrical configuration of the region of the conceptual model (BRAGFLO) to which the data are applied differs from the assumptions of the model used to generate it, scaling of the data is considered adequate to justify its use. The principal differences are that the geometry of the waste regions and the mechanical material response functions used to generate the data are much more detailed in the creep closure model than the BRAGFLO model that receives the data.

Repository Fluid
Flow

1. Model Name

Repository Fluid Flow

2. Responsible Contact

P. Vaughn

3. Model Description and References

The first principle in the conceptual model for fluid flow in the repository is that gas and brine can both be present and mobile (two-phase flow), governed by conservation of energy and mass and by Darcy's Law for their fluxes. Consistent with typical concepts of two-phase flow, the phases can affect each other by impeding flow due to partial saturation (relative permeability effects) and by affecting pressure due to capillary forces (capillary pressure effects).

The geometry of two regions in the repository is specified to be consistent with an assumption about the types of flow that can occur there. In the separate panel, the center of which can be intruded by a borehole, it is assumed that flow between the borehole and panel is convergent or divergent. This creates a "neck" in the separate panel. If flow crosses this panel laterally, it will converge to pass through the neck and then diverge. Because of the permeability contrasts in the system and time scales involved, it is not expected that the neck in the panel is significant, especially with the pillars in the panel removed. Similarly, in the operations region the shaft is assumed to have convergent or divergent flow, creating a neck. This is also assumed to have an insignificant effect on flow that might cross the operations region.

Gas generation is sensitive to the quantity of liquid in contact with metal. Because of this, the conceptual model for the distribution of fluid in the repository is considered sensitive. However, the distribution of fluid in the repository is not possible to determine realistically. For example, capillary action can create wicking that would increase the overall region in which gas generation occurs, but this cannot be modeled without undesirable effects on the duration of the model simulations. Therefore, it is conceptualized only for the purposes of gas generation that whatever brine is in the repository is distributed to an extent greater than actually estimated by the Darcy flow models used and values of parameters chosen.

4. Model Purpose

This model represents the long-term behavior of flow of liquid and gas in the repository and its interaction with other regions in which fluid flow may occur, such as the Salado, shafts, or exploration borehole. This model is not used to represent the interaction of fluids in the repository during drilling with a borehole.

5. Principal Parameters and Relationship among Parameters Defined by the Model

Darcy flow for two phases implies certain important parameters. Some principal parameters relate to the properties of the fluid, others to the rock. Fluid properties in the Darcy flow model used for WIPP are its density, viscosity, and compressibility. Rock properties in Darcy flow models are porosity, permeability, and pore compressibility. Other parameters are required to describe the interactions or interference between the two phases present in the model, gas and brine, because they can occupy the same pore space. In the WIPP application of these models, compressibility of both the liquid and rock are related to porosity through a dependence on pressure. Fluid density, viscosity, and compressibility are often closely related to fluid composition, pressure, and temperature. For the WIPP, fluid viscosity is a function of pressure, but its density and compressibility are held constant. Fluid composition for the purposes of modeling flow and transport is assumed to be constant.

Repository Fluid Flow. The flow of brine and gas in the repository is assumed to behave as two-phase, immiscible, Darcy flow. BRAGFLO is used to simulate brine and gas flow in the repository and to incorporate the effects of disposal room closure and gas generation. Fluid flow in the repository is affected by the following factors:
- the geometrical association of pillars, rooms, and drifts; panel closure due to creep; and possible borehole locations;
- the varied properties of the waste areas resulting from creep closure and heterogeneous contents;
- flow interactions with other parts of the disposal system; and
- reactions that generate gas.

Creep closure changes disposal region porosity. Depending on material properties and conditions, brine may flow into the disposal region by moving down shafts and through the DRZ or operations region or, during disturbed conditions, through a borehole. Brine contained in the Salado may flow to the waste disposal region because of pressure gradients created by the excavation. Brine flow into the repository may be reduced as repository pressure increases, and brine may be expelled from the repository if pressure exceeds brine pressure in the immediately surrounding rock or borehole. Large quantities of gas may be generated as waste decomposes, causing a pressure increase. Gas may flow away from the waste into lower-pressure areas, which may include disturbed areas surrounding the repository, the interbeds, the shafts, or an intrusion borehole. Gas flow into intact, halite-rich rock is not expected to be important because of the expected high threshold pressure of halite.

To account for parameter and conceptual model uncertainty in estimating repository fluid flow, the DOE has incorporated reasonably conservative assumptions and modeling approaches to ensure that the four primary factors affecting fluid flow listed above are not underestimated. The

conservative assumptions and modeling approaches used in the performance assessment are discussed for each factor below.

Repository Geometry. The BRAGFLO model of the repository includes a waste disposal panel, panel closures, the panels and access drifts in the rest of the waste disposal region, the operations region, and the experimental region at the north end of the repository. For each region represented, the BRAGFLO model of the repository preserves the true excavated volume. Lateral dimensions have been determined to preserve volume and retain important cross-sectional areas and distances between defined regions. These simplifications are conservative with respect to fluid contact with the waste, which is a critical factor in determining the quantity of actinides mobilized in the aqueous phase. The simplifications are conservative for two reasons. First, all pillars have been removed from panels, resulting in homogeneous waste regions through which fluid can flow directly. Second, the panels in the rest of the repository have neither pillars nor closures, resulting in a very large region of homogeneous waste that is assigned a high permeability. Tests on simulated waste compacted under a lithostatic load (Luker et al., 1991) have shown that material permeabilities change from about 10^{-12} to 10^{-16} m^2. For performance assessment calculations, the waste disposal region is assigned a constant permeability of 1.70×10^{-13} m^2, a value representative of unconsolidated waste. This permeability facilitates fluid flow under low hydraulic gradients, which tends to increase potential releases.

Modeling of flow within the repository is based on homogenizing the room contents into relatively large computational volumes. The approach ignores heterogeneities in disposal room contents that may influence gas and brine behavior in the room by causing fluid flow among channels or preferential paths in the waste, bypassing entire regions. Isolated regions could exist for several reasons:
- they may be isolated by low-permeability waste barriers;
- connectivity with the interbeds may occur only at particular locations within the repository; or
- the repository dip may promote preferential gas flow in the upper regions of the waste.

The adequacy of the homogenization approach was examined in a screening analysis (FEP: DR-6, see records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6"). To address room heterogeneity, this analysis used an additional parameter in BRAGFLO to specify the minimum active (mobile) brine flow saturation (pseudo-residual brine saturation). Above this saturation, the normal descriptions of two-phase flow apply (i.e., either the Brooks/Corey or van Genuchten/Parker relative permeability models). Below this minimum, brine is immobile, although it is available for reaction and may still be consumed during gas-generation reactions. The assumption of a minimum saturation limit is justified based on the presumed heterogeneity of the waste and the fact that the repository dips slightly. The minimum active brine saturation was treated as an uncertain parameter and sampled uniformly between values 0.1 and 0.8 during the analysis. This saturation limit was applied uniformly throughout the disposal room in order to bound the impact of heterogeneities on flow (Appendix 2 of the records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6"). Results of this analysis showed that differences in releases to the accessible environment between the baseline case (homogenization) and puddling case (isolated regions of brine saturation) are minor, with the baseline model predicting consistently higher releases.

Waste Properties Resulting From Closure. The waste disposal region is assigned an initial porosity of 84.8%. The porosity is adjusted during the simulation based on the porosity surface calculated by SANTOS to account for pressure-dependent consolidation of the waste by creep closure. As noted above, the waste disposal region is assigned a constant high permeability of 1.70 x 10^{-13} m^2, a value representative of unconsolidated waste.

The experimental and operations regions are represented in performance assessment by a fixed porosity of 18.0% and a permeability of 10^{-11} m^2. This combination of low porosity and high permeability will conservatively overestimate fluid flow through these regions and minimize the capacity of these regions to store fluids, thus maximizing releases to the environment. This conclusion is based on a screening analysis (FEP: DR-7; records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6") that examined the importance of permeability varying with porosity in closure regions (waste disposal region, north end, and hallways). To perform this analysis, a model for estimating the change in permeability with porosity in the closure regions (waste disposal region, north end, and hallways) was implemented in BRAGFLO (Appendix 2 of the records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6"). A series of BRAGFLO simulations was performed to determine whether permeability varying with porosity in closure regions could enhance contaminant migration to the accessible environment. Two basic scenarios were considered in the screening analysis, undisturbed performance and disturbed performance. To assess the sensitivity of system performance on dynamic permeability in the closure regions, conditional complementary cumulative distribution functions (CCDFs) of normalized contaminated brine releases to the Culebra after human intrusion via the shaft system, as well as releases to the subsurface boundary of the accessible environment, were constructed and compared with the corresponding baseline model CCDFs. The baseline model treated permeabilities in the closure regions as fixed values. Results of this analysis showed that the inclusion of dynamic closure of the waste region, north end, and hallways in BRAGFLO results in computed releases to the accessible environment that are essentially equivalent to the baseline case.

The panel closures are represented with a porosity of 7.5% and a permeability of 10^{-15} m^2. The permeability is consistent with the corresponding properties of the DRZ.

Because two-phase relationships have not been measured for waste, performance assessment determines a range of possible two-phase conditions for the repository by applying Latin hypercube sampling (LHS) to either the Brooks-Corey or van Genuchten-Parker two-phase equations.

Flow Interactions with Other Parts of the Disposal System. In past calculations, the dynamic effect of halite creep and room consolidation on room porosity was modeled only in the waste disposal regions. Other parts of the repository, such as the experimental region in the north end and the hallways, were modeled assuming fixed (invariant with time) properties. In these regions, the permeability was held at a fixed high value representative of unconsolidated material, while the porosity was maintained at relatively low values associated with highly consolidated material. It was assumed that this combination of low porosity and high permeability would conservatively overestimate flow through these regions and minimize the capacity of this material to store fluids, thus maximizing the release to the environment. To examine the validity of this assumption, a

screening analysis (FEP: DR-3, see records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6") evaluated the effect of including closure of the north end and hallways. In this analysis, consolidation of the north end and hallways was implemented in BRAGFLO by relating pressure and time to porosity using a porosity-surface method. The porosity surface is a look-up table within BRAGFLO that relates cavity closure (void volume) to time and pressure for various gas generation histories. This porosity surface is calculated independently of BRAGFLO by the computer code SANTOS (Butcher et al., 1991). The porosity surface for the north end and hallways differs from the one used for consolidation of the disposal room and is based on an empty excavation (memo from Stone and Arguello to Butcher entitled "Porosity Surface Generation for a Disposal Room Without Crushed Salt Backfill," dated 2/2/95). Results of the analysis showed that the assumption is valid: including closure of the north end and hallways and consequent reduction of porosity results in overall lower computed releases to the accessible environment than the baseline releases computed with time-invariant high permeability and low porosity.

Gas Generation. Gas generation affects repository pressure, which in turn is an important parameter in other processes such as two-phase flow, creep closure, and interbed fracturing. Gas generation processes considered in performance assessment calculations include anoxic corrosion and microbial degradation. Radiolysis is excluded from performance assessment calculations on the basis of laboratory experiments and a screening analysis (FEP: GG-1, see records package entitled "FEPs Screening Analysis for FEPs GG-1 and S-1") that concluded that radiolysis does not significantly affect repository performance.

An average stoichiometric process model is used in BRAGFLO to estimate disposal region gas generation by anoxic corrosion and microbial degradation of cellulosics, including plastics and rubbers. In calculating repository pressure and gas flow, the generated gas is assumed to be H_2. This model requires several assumptions about the chemical conditions of the disposal region. In the average stoichiometric model, gas is assumed to be generated at a rate dependent on the availability of brine in a BRAGFLO waste region computational cell. This model is based on experimental corrosion and biodegradation data. The data were used to develop ranges of possible gas-generation rates under inundated and humid conditions. A linear interpolation method is used to combine humid and inundated rates based on the effective liquid saturation. These ranges are sampled using LHS to account for uncertainties in humid and inundated rates. To account for uncertainties in long-term gas generation, only half the realizations include biodegradation, and only one quarter include biodegradation of rubbers and plastics.

In modeling gas generation, the effective liquid in a computational cell is the computed liquid in that cell plus an adjustment to account for the uncertainty associated with wicking by the waste. Capillary action (wicking) is the ability of a material to carry a fluid by capillary forces above the level it would normally seek in response to gravity. Since the current gas-generation model computes substantially different gas-generation rates depending on whether the waste is wet or merely surrounded by water vapor, the physical extent of wetting could be important. A screening analysis (FEP: DR-2, see records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6") examined wicking and concluded that it should be included in performance assessment calculations. The baseline gas-generation model in BRAGFLO accounts for corrosion

of iron and microbial degradation of cellulosics. The net reaction rate of these processes depends directly on brine saturation: an increase in brine saturation will increase the net reaction rate by weighting the inundated portion more heavily and the slower humid portion less heavily. To simulate the effect of wicking on the net reaction rate, an effective brine saturation, which includes a wicking saturation contribution, is used to calculate reaction rates rather than the brine saturation. To account for uncertainty in the wicking saturation contribution, this contribution was sampled from a uniform distribution of range from 0.0 to 1.0 for each BRAGFLO simulation in the analysis.

References:

Butcher, B.M., T.W. Thompson, R.G. VanBuskirk, and N.C. Patti. 1991. *Mechanical Compaction of Waste Isolation Pilot Plant Simulated Waste*. SAND90-1206. Albuquerque, NM:Sandia National Laboratories.

Key, S., et al. *Background and Basis for the Fluid Flow Model Incorporated in BRAGFLO for Representing Pore Pressure-Induced Alterations in Permeability and Porosity in the Anhydrite Interbeds Above and Below the WIPP Repository Horizon.* SAND94-0381. Albuquerque, NM:Sandia National Laboratories..

See also:

FEPs Screening Analyses, Records Package, SWCF:1.1.6.3:PA:NG:TSK:DR2,DR3,DR6,DR7, and S6 FEPs Screening Analyses,

FEPs Screening Analyses, Records Package, SWCF:1.1.6.3:PA:NG:TSK: GG1 and S7

Gas Generation

1. Model Name

Gas Generation

2. Responsible Contact

L. Brush

3. Model Description and References

Gas will be produced in the repository by a variety of chemical reactions—principally those between brine, metals, microbes, cellulosics and similar materials, plastics, and rubber materials— and by liberation of dissolved gases to the gaseous phase. The processes assumed for long-term performance are anoxic corrosion of metals in the waste and waste containers and microbial degradation of cellulosic waste. Anoxic corrosion reactions between brine and steel are expected to occur and produce H_2; they are included in the conceptual model. Microbial degradation of cellulosics might occur. If it does, it may produce various gases, primarily CH_4, CO_2, N_2, and H_2S. However, by reaction with the MgO backfill that will be emplaced to control the chemistry of the repository, CO_2 produced by microbial degradation will be removed from the gaseous phase. (Because of the volume and properties of the material emplaced, this backfill will not have any effect on creep closure or waste encapsulation.) Other gases produced by microbial degradation are considered to be insignificant compared with the quantity of gas produced by anoxic corrosion. Thus the conceptual model for gas generation is that anoxic corrosion of steel will produce H_2; microbial degradation of cellulosics, plastics, and rubbers might occur and might produce gas, but the CO_2 is rapidly removed by reaction with MgO backfill.

In the conceptual model, the rate of gas production in the repository by anoxic corrosion can be limited by several factors. Anoxic corrosion cannot occur unless liquid is present and in contact with steel. Because anoxic corrosion consumes steel, the rate of gas production can be limited by the quantity of steel left in the repository. Because corrosion is a surface reaction, it proceeds at quantifiable rates per unit surface area of steel. In addition, anoxic corrosion consumes water. Because of these factors, the rate of gas generation in the repository can vary through time as conditions change. It is assumed that anoxic corrosion can occur in the repository as soon as the shafts are sealed for as long as brine is present.

Microbial degradation of cellulosics, plastics, and rubbers is limited by several factors, chiefly the viability of microbes in the repository. Whether microbes degrade plastics and rubbers is also important. Microbial degradation requires liquid to be present, but due to uncertainty is assumed neither to consume nor produce water.

Radiolysis has been considered but has been demonstrated by laboratory experiment and model calculations to be insignificant.

Oxygen will be present in the panels when panel closures are emplaced and in the repository when shaft seals are constructed. Until gaseous oxygen is consumed, oxic reactions will occur in the waste. This process cannot persist for long due to the rate that oxic reactions proceed and the limited quantity of oxygen present. Oxic reactions are not considered in the conceptual model for gas generation in the repository because it is insignificant compared with the potential for gas generation from anoxic reactions.

Addition of a MgO backfill significantly reduces the impact of microbial generation of CO_2. As discussed in Section 6.4.3.4 of the CCA, the MgO backfill will react with carbon dioxide produced by microbial degradation and remove it from the gaseous phase.

4. Model Purpose

This model represents the possible generation of gas in the repository by corrosion of steel and microbial degradation of cellulosics, plastics, and rubbers.

5. Principal Parameters and Relationship among Parameters Defined by the Model

Because the conceptual model discusses the general processes and interactions assumed to occur without direct reference to the mathematical equations used, no parameters are defined by this conceptual model. The mathematical model used to implement it, the Average Stoichiometry Model, is documented in Section 6.4.3.3 of the CCA and Appendix BRAGFLO, as well as in memoranda attached to this section. The most important parameter in the Average Stoichiometry Model is the rate at which gas generation occurs with brine and steel present, because this is the principal control on the total quantity of gas generated. The assumptions made about the principal reactions and their stoichiometry (documented in an attached memorandum) are also important, however, because they affect the quantity of gas created per unit quantity of steel and water reacted.

The feedback between the gas generation conceptual model and the repository fluid flow conceptual model is important to understand. Gas generation cannot continue for long with the low initial quantity of liquid present in the waste, as specified by the Waste Acceptance Criteria (WAC). For gas generation to occur, liquid must flow into the repository; for gas generation to be sustained, liquid consumed by gas generation must be replenished. Gas generation, however, tends to increase repository pressure and to keep liquid from flowing into it. Thus the rates at which various processes proceed are important in determining the conditions of the repository. There is important feedback as well between the gas generation model and other conceptual models through pressure effects, such as those calculating creep closure (Section 6.4.3.1), interbed fracturing (Section 6.4.5.2), two-phase flow (Section 6.4.3.2), and the radionuclide release associated with spalling during an inadvertent drilling intrusion (Section 6.4.7).

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Single-process laboratory studies of anoxic corrosion of steels and Al-based materials by R. E. Westerman and his colleagues at Pacific Northwest Laboratory (PNL) from

November 1989 through September 1995 have shown that the factor with the greatest effect on the rate of H_2 generation by anoxic corrosion is the quantity of brine in WIPP disposal rooms. This is because anoxic corrosion occurs rapidly under inundated conditions, but not at all under humid conditions. The pressure difference between WIPP disposal rooms and the far field and the porosity of the room contents also affect the extent of brine inflow and outflow and, hence, the anoxic-corrosion rate. Because the average-stoichiometry model (the gas-generation model used for performance assessment (PA) calculations) is incorporated in the multi-phase flow code BRAGFLO, gas generation is coupled with brine and gas inflow and outflow. Moreover, because BRAGFLO uses a porosity surface to simulate room closure (Butcher and Mendenhall, 1993), it also couples gas generation to room closure. Telander and Westerman (1993) and subsequent studies of anoxic corrosion at PNL have shown that pH, pressure, and the composition of the gaseous phase also affect the H_2-generation rate.

The greatest uncertainty in modeling gas generation in WIPP disposal rooms is whether microbial gas generation will occur and, if so, to what extent it will occur and what its effects will be. Brush (1995) described the following sources of microbial uncertainty in detail:
- whether microorganisms capable of carrying out the potentially significant respiratory pathways identified by Brush (1990) (denitrification, SO_4^{2-} reduction, and methanogenesis) will be present when the repository is filled and sealed;
- whether these microbes will survive for a significant fraction of the 10,000-year period of performance of the repository;
- whether sufficient H_2O will be present in the waste or brine;
- whether sufficient electron acceptors (oxidants) will be present and available;
- whether enough nutrients, especially N and P, will be present and available;
- whether microbes will consume significant quantities of plastics and rubbers during the 10,000-year period of performance of the repository; and
- the stoichiometry of the overall reaction for each significant respiratory pathway, especially the number of moles of electron acceptors, nutrients, gases, and H_2O consumed or produced per mole of substrate consumed.

With regard to the first five of these uncertainties, Brush (1995) concluded that, although significant microbial gas production is possible, it is by no means certain. Therefore, he estimated that the probability of significant microbial gas generation in WIPP disposal rooms is 50%, and that the probability that microbes will consume all of the plastics and rubbers in the repository after they consume all of the cellulosics is also 50%.

Single-process laboratory studies of microbial consumption of cellulosics by A. J. Francis and his colleagues at Brookhaven National Laboratory (BNL) from May 1991 through September 1995 showed that if significant microbial activity occurs, the factor with the greatest effect on the microbial gas-generation rate is the quantity of brine in the repository (see Francis and Gillow, 1994). This is because microbial gas generation occurs rapidly under inundated conditions, but not at much lower rates under humid conditions. Francis and Gillow (1994) also found that inoculation with halophilic microbes from the WIPP Site and vicinity, amendment with NO_3^- (an electron acceptor), amendment with nutrients, and addition of bentonite (a previously proposed backfill material) affect the rate or extent of microbial gas generation. Other

factors that could affect the rate or extent of microbial gas generation, but which Francis and Gillow (1994) did not quantify, are the pH; the dissolved or suspended concentrations of actinides or other heavy metals, which could inhibit or preclude microbial activity; and the concentrations of microbial byproducts, which could inhibit or preclude additional microbial activity. However, if microbial activity occurs, high pressure will not preclude or even inhibit it significantly, even when it increases to 150 atm (lithostatic pressure at the depth of the repository).

Data summarized by Molecke (1979) imply that radiolysis of cellulosics, plastics, and rubbers will not be a significant, long-term gas-generation process in WIPP disposal rooms. ("Radiolysis" here refers to α radiolysis, the chemical dissociation of molecules by α particles emitted during the radioactive decay of the actinide elements in TRU waste. Because molecular dissociation caused by other types of radiation will be insignificant in a TRU-waste repository such as the WIPP, this paper considers only α radiolysis.) Based on calculations using the results of laboratory studies of brine radiolysis carried out for the WIPP by Reed et al. (1993), on estimates of the quantities of brine that could be present in the repository after filling and sealing, and on estimates of the solubilities of Pu, Am, Np, Th, and U summarized by Trauth et al. (1992), Brush (1995, Appendix E) concluded that radiolysis of H_2O will not significantly affect the overall gas or H_2O content of the repository. However, this conclusion is very sensitive to the dissolved and suspended concentrations of these actinides, and it might have to be reevaluated using the results from the Actinide Source Term Program that will actually be used in the PA calculations to support the CCA.

7. FEPs Associated with Model Development

GG-1, effects of brine radiolysis on the gas content of WIPP disposal rooms;
GG-2, comparison of the average-stoichiometry and the reaction-path gas-generation models;
GG-3, chemical (especially pH) changes caused by gas generation;
GG-4 and/or RNT-25?, effects of thermal gradients on the brine content of the repository;
GG-5, effects of radiogenic He production on the gas content of the repository;
GG-6, chemical changes caused by corrosion;
GG-7, effects of chemical reactions on the temperature of the repository;
GG-8 and/or RNT-26?, effects of radioactive gases on release of radionuclides from the repository;
GG-9, effects of temperature on microbial gas generation;
GG-10, effects of pressure on microbial gas generation;
GG-11, effects of radiolysis of combustibles on the gas content of WIPP disposal rooms;
GG-12, DR-15, DR-16, and/or RNT-25?, effects of galvanic coupling on corrosion;
GG-13, DR-15, DR-16, and/or RNT-25?, effects of electrochemical gradients on corrosion;
GG-14, effects of biofilms (on corrosion?).

8. History of Model Development

The WIPP Project performed laboratory studies of gas generation during the late 1970s to support the development of transuranic (TRU) waste-acceptance criteria (Molecke, 1978, 1979;

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Sandia Laboratories, 1979). The Project did not develop a gas-generation model in the late 1970s. For the most part, these laboratory studies comprised single-process experiments (one gas-generation process studied at a time) on microbial activity and radiolysis with nonradioactive and some radioactive simulated TRU waste. There was very little work on anoxic corrosion. Based on laboratory measurements on samples obtained by drilling from the surface, the permeability of the Salado Formation appeared to be high enough for rapid migration of gas from the repository, even given the highest gas-generation rates summarized by Molecke (1979). Furthermore, EPA regulations for chemically hazardous waste constituents did not apply at the time these studies were conducted. Therefore, the Project terminated these studies of gas generation in 1979.

In 1987, preliminary performance-assessment calculations on the effects of human intrusion identified inflow of intergranular Salado brine as a concern for the long-term performance of the repository. In early 1988, Sandia National Laboratories began to examine the possible effects of processes such as anoxic corrosion of steels and microbial degradation of cellulosics on the H_2O content of WIPP disposal rooms. Brush and Anderson (1989a) concluded that these processes could affect the H_2O content as significantly as brine inflow. Furthermore, they concluded that these processes could also produce significant quantities of gas. Meanwhile, in situ measurements in the WIPP underground workings revealed that the permeability of the Salado was much lower than believed in the late 1970s.

Systems analysis carried out by Lappin et al. (1989) to support the 1990 Supplemental Environmental Impact Statement, which used gas-generation assumptions from Brush and Anderson (1989a, 1989b, and 1989c), the rates-and-potentials gas-production model of Lappin et al. (1989), and new in situ permeabilities, demonstrated that gas would affect the overall performance of the repository if present in significant quantities.

Therefore, the Project restarted laboratory studies of gas generation in February 1989. These studies have comprised mainly single-process experiments on anoxic corrosion, microbial activity, and radiolysis, mostly with nonradioactive, simulated contact-handled (CH) TRU waste (Brush, 1990; Brush et al., 1991a, 1991b, 1993; Reed et al., 1993; Telander and Westerman, 1993; Francis and Gillow, 1994).

The Project has also developed three gas-generation models since 1989 (Brush, 1995). For their 1989 systems analysis, which demonstrated that gas will affect repository performance, Lappin et al. (1989) developed the rates-and-potentials gas-generation model. WIPP Performance Assessment Division (1991) developed the average-stoichiometry gas-generation model and incorporated it into BRAGFLO, which also simulates room closure. Incorporation of the average-stoichiometry model into BRAGFLO thus coupled this gas-generation model with the hydrologic and geomechanical models used for PA. In 1992, work began on the reaction-path gas-generation model, which includes more gas-generation processes than the average-stoichiometry model and the interactions among these processes (Brush et al., 1994). Brush (1995) recommended replacing the average-stoichiometry model in BRAGFLO with the reaction-path model. However, in November 1995, the WIPP Project decided to terminate all work on the reaction-path model and to continue to use the average-stoichiometry model in

BRAGFLO. Brush et al. (1995, see attached memorandum) explained the reasons for abandoning the reaction-path model.

9. Information Supporting Model Choice and Confirmation

Lappin et al. (1989) developed the rates-and-potentials gas-generation model prior to the restart of laboratory studies of gas generation. They used previously published information and assumptions and estimates of gas-generation rates provided by Brush and Anderson (1989a, 1989b, 1989c) to develop this model.

WIPP Performance Assessment Division (1991) and Brush et al. (1994) developed the average-stoichiometry and the reaction-path gas-generation models, respectively, based on the results of the single-process laboratory studies that were restarted in 1989. However, although these laboratory studies considered only one gas-generation process at a time (anoxic corrosion, microbial activity, or radiolysis), they did, at least to some extent, simulate some of the possible interactions between these processes. For example, the study of anoxic corrosion by Telander and Westerman (1993) considered the effects of the microbially produced gases CO_2 and H_2S on corrosion, and Brush et al. (1994) included passivation of steels and other Fe-based metals by CO_2 and H_2S in the reaction-path model.

10. Validity and Completeness

Soon after Brush and Anderson reraised the gas issue in the late 1980s, the WIPP Project decided to validate laboratory studies of gas generation and the models based on them with studies of gas generation by actual TRU waste. Therefore, the WIPP Project started to plan large-scale, multi-process tests with CH TRU waste in the WIPP underground workings (Molecke, 1990a, 1990b; Molecke and Lappin, 1990; Lappin et al., 1991). On October 21, 1993, the DOE canceled the bin and alcove tests prior to their initiation in the WIPP underground workings. This decision was based, at least in part, on the results of the Independent Technical (Red Team) Review of these tests (U.S. Department of Energy Office of Environmental Restoration and Waste Management, 1993). The DOE also announced that an Enhanced Laboratory Program (ELP) would replace the bin and alcove tests.

In late 1993, the Project began planning the ELP. At that time, plans included both a multi-process study with radioactive (Pu-doped) simulated waste (initially called the ELPSPUD) and multi-process tests with actual CH TRU waste (initially referred to as the ELPSAT). The Project planned to perform the study with radioactive, simulated waste at Argonne National Laboratory (ANL) - East. The main objective of this study would have been to determine whether the average-stoichiometry and the reaction-path gas generation models, based on the results of single-process studies, could predict the results of multi-process experiments. However, in May 1995 the Project terminated the study prior to obtaining any data (Shephard, 1995. This discussion also pertains to the decision to terminate the single-process studies by September 1995.) The multi-process study with actual CH TRU waste is now under way at ANL - West and will continue for about two to five years. However, these tests started after development of the

average-stoichiometry model was frozen in September 1995 and after gas-generation data were submitted to PA in January 1996.

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1. Model Name

Chemical Conditions and Dissolved Actinide Source Term Conceptual Models

The dissolved actinide source term (AST) model is composed of several conceptual "submodels." The solubility submodel is the Fracture-Matrix-Transport (FMT) model that is based on the Pitzer semi-empirical activity coefficient model of the thermodynamics of highly concentrated electrolytes. This model uses appropriate adaptations of the Harvie-Møller-Weare/Felmy-Weare (HMW/FW) data base. FMT parameters are fitted using the code NONLIN, which calculates the Pitzer parameters. As used in the AST, there are no redox equations implemented in FMT; instead an oxidation state analogy and an oxidation state distribution "submodel" are used.

To estimate concentrations of actinides in solution, the model is implemented as follows. For a particular brine at a particular organic ligand concentration, pmH and CO_2 fugacity, the solubility of the actinide oxidation states is modeled by FMT. The oxidation state distribution submodel determines the relevant oxidation state for each actinide, and each oxidation state is assigned the appropriate solubility, as described in Section 6.4.3.6.

2. Responsible Contacts

FMT and database model development: C. F. Novak
Development of organic ligand input to FMT: R. A. Moore
Development of oxidation state distribution: R. F. Weiner
Program integration: R. V. Bynum
Development of interface with performance assessment: R. F. Weiner and C. T. Stockman
NONLIN: A. R. Felmy (PNNL) and C. F. Novak (SNL)
Development of WIPP relevant brine pmH and f(CO_2): Y. Wang

3. Model Descriptions and References

The conceptual model for chemical conditions in the repository includes variability in brine composition as a major factor and assumes the addition of an MgO backfill with the waste. The chemical environment will be reducing due to the presence of steel, and possibly microbes, and the reactions they support. Given reducing conditions, MgO backfill, and the brine types present naturally in the disposal system, the repository will have low CO_2 fugacity and alkaline conditions (pH between 9 and 10). The principal brine types are Castile and Salado; in Salado brine, repository conditions will be slightly more acidic.

In the conceptual model, actinide solubilities depend on the pH and other criteria such as organic ligand concentrations and the stability of possible oxidation states in repository conditions.

The determination of repository chemical conditions and actinide solubilities in them has been the subject of experiments and numerical simulation. Much of the discussion in this section addresses the manner in which actinide solubilities are used in performance assessment.

FMT. The FMT code uses experimentally developed Pitzer parameters to calculate concentrations of constituents of highly concentrated electrolyte solutions, including dissolved actinides, in equilibrium with solubility-controlling solids. It is used to calculate actinide solubilities (equilibrium dissolved concentrations) in the WIPP because available parameters reflect the chemical conditions that will prevail in the WIPP repository.

References:

Novak, C. F. and K. E. Roberts. 1994. "Thermodynamic Modeling of Neptunium (V) Solubility in Na-CO$_3$-HCO$_3$-Cl-ClO$_4$-H-OH-H$_2$O Systems" *Symposium on the Scientific Basis for Nuclear Waste Management, Kyoto, Japan, October 21-26.*

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HMW/FW. HMW/FW is a parameterization of the Pitzer formalism for calculating activity coefficients in concentrated electrolyte solutions. HMW/FW provides a database for describing solubility behavior in the Na-K-Mg-Ca-H-Cl-SO$_4$-OH-HCO$_3$-CO$_3$-CO$_2$-B-H$_2$O system, which includes the significant inorganic constituents of WIPP brines.

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Pitzer, K. S. 1991. *Activity Coefficients in Electrolyte Solutions.* Boca Raton, FL: CRC Press, Chapters 1 through 3.

NONLIN. NONLIN calculates parameters for FMT using a nonlinear least-squares program in combination with a program that minimizes the Gibbs free energy (chemical potential).

References:

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Oxidation State Distribution. The oxidation state distribution in the WIPP is modeled from data obtained in experiments by the DOE at Los Alamos National Laboratory and Pacific Northwest National Laboratory, and from the existing liturature.

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See also:

Appendix SOTERM

4. Model Purpose

The purpose of the dissolved AST model is to predict equilibrium dissolved concentrations of the actinides thorium, uranium, neptunium, plutonium, americium, and curium under the range of chemical conditions that could occur in the WIPP repository in the presence of brines. Dissolved actinides can be transported by the solvent (brine) out of the repository under various human-intrusion scenarios.

5. Principal Parameters and their Interrelationships

The FMT code calculates the solubility of species in equilibrium with a solubility-controlling solid in strong electrolyte solutions. It is an application of the Pitzer formalism that describes the thermodynamics of concentrated electrolyte systems. The Pitzer formalism recognizes that ion-ion interactions are more important to thermodynamics in concentrated strong electrolyte solutions than in dilute solution. Both Castile brine and Salado brine are highly concentrated (~5 M to 6 M) salt solutions, making the Pitzer formalism is applicable. Choice of the Pitzer formalism is discussed in Sections 8 and 9.

Activity coefficients in such concentrated solutions may be expressed as a function of the ion-ion interactions. Some parameters of this function depend strongly on the ionic strength and may be determined experimentally. The HMW/FW data base is an experimentally determined set of parameters for calculating solubilities in concentrated electrolyte solutions. Where appropriate parameters already existed in the HMW/FW data base, they have been used in FMT calculations for the WIPP. Additional parameters, most notably for the actinide ions and for the organic ligand compounds expected in the WIPP inventory, have been determined from experimental data using the NONLIN code.

The FMT calculations were done for three actinides that were analogs for the +3, +4, and +5 oxidation states, with and without organic ligands. Five organic ligands are capable of

significantly enhancing dissolved actinide concentrations, are potentially present in the repository, and are generally representative of any organic ligand that could be present in the WIPP: acetate, citrate, oxalate, lactate, and EDTA. Four of these (acetate, citrate, oxalate, and EDTA) were identified in the waste inventory of the WIPP (Watkins, 1996) as the only water-soluble organic ligands present in significant quantities. Lactate was not included because none was identified in the inventory, and estimating its concentration resulting from both production and consumption by microbes is not possible. In calculations including organic ligands, all four of the water-soluble organic ligands identified in the WIPP inventory were included together at the expected concentrations, so that competition among complexing sites could be examined. Calculations were done separately for Salado and Castile brines, using the brine formulations given by Brush (1990, pp. 17-28). The FMT output is the equilibrium solubility of the actinide as a function of the repository conditions.

Solubilities were modeled by FMT for actinides in particular oxidation states: Am(+3), Th(+4), and Np(+5). Because actinides in the same oxidation state exhibit similar chemical behavior, these FMT models are applied to all actinides in that particular oxidation state; e.g., the Am(+3) FMT model applies to Pu(+3) and Cm(+3); and the Np(+5) model applies to Pu(+5). Although U(+4) is not as close an analog to Th(+4) as Pu(+3) is to Am(+3), the analogy was extended to the Th(+4) model, resulting in some uncertainty, as discussed in Section 6.

As described in Section 6.4.3.5 of the CCA, the solubilities modeled using FMT are combined with the oxidation states of each actinide to give the total concentration of the dissolved actinide in the WIPP brine. The oxidation states expected to be stable were determined by a study of the literature and by the WIPP experimental program. Redox reactions between actinides are not expected to be important, because actinide concentrations will be much lower than concentrations of other constituents of the brine. For three of the actinides, the analysis shows that there will only be one stable oxidation state: Am(+3), Cm(+3), and Th(+4). For the other three, two oxidation states are possible in the expected range of conditions: U(+4) and U(+6), Np(+4) and Np(+5), and Pu(+3) and Pu(+4). The uncertainty in the effective WIPP repository redox state was incorporated into the PA by use of the solubilities of the lower oxidation state in half of the realizations in the PA and of the higher oxidation state in the other half of the realizations for these actinides. Sufficient Pitzer parameters for the +6 oxidation state have not been determined, so empirically determined solubilities will be used for U(+6).

The initial implementation of the dissolved actinide source term (coded in the fall of 1995) included a preliminary source term code that read BRAGFLO output and calculated time-dependent solubilities. CO_2 generation competed with $Ca(OH)_2$ (from waste forms treated with Portland cement) dissolution and brine flows to establish a pmH between 4 and 13. The $f(CO_2)$ ranged from 55 atm to 10^{-13} atm. The addition of MgO as a backfill is expected to buffer both the pmH and $f(CO_2)$ to the values determined by the equilibrium between $MgCO_3$ and $Mg(OH)_2$ in each possible WIPP brine. Examination of the range of the relative amounts of brines and $Ca(OH)_2$ expected in the WIPP repository showed that only very rarely could the $CaCO_3$ - $Ca(OH)_2$ buffer determine the pmH and $f(CO_2)$ (Wang 1996). Therefore only two FMT calculations were required for the main compliance calculations, one for Castile brine and one for

Salado brine. To support sensitivity analysis, additional calculations are also under way to provide solubilities in the absence of added MgO.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The uncertainties associated with the dissolved actinide source term include both uncertainties in the experimental data produced by the AST program and uncertainties on how to apply the experimental results to the WIPP. The first of these has been estimated to be relatively small. It has been demonstrated (Novak, 1995; Novak and Roberts, 1996) that uncertainties in the solubility data and the resulting Pitzer coefficients implemented in FMT result in uncertainty in the model predictions of an order of magnitude or less for the sets of chemical conditions that have been tested. This is also evident when the data of Kim et al. (1985) are compared with FMT model results. The magnitude of uncertainty arising from the method of application of the FMT models to the WIPP is harder to estimate.

Uncertainties arising from the application of the FMT model are connected with four issues:
* whether dissolution/precipitation steady state is obtained;
* extrapolation outside the region for which FMT data were collected;
* use of the oxidation state analogy; and
* chemical conditions at the WIPP.

Dissolution and Precipitation. The Project assumes that the time required for brine to flow through the repository and up a borehole is long enough to establish chemical equilibrium or steady state between the solubility-controlling solids and the solution. In the present conceptual model of the repository, brine reservoir, and intrusion borehole, the repository will contain brine for several hundred years before there is significant movement of brine up the borehole. During the years soon after closure, the chemistry within the repository will rapidly change from that dominated by ventilation air and high nitrate concentrations to that dominated by reduction of all oxidized species by iron metal and possibly the digestion of cellulose by microbes. Supersaturation above the solubilities seen in the week-long to month-long experiments of the AST program will be highly unlikely: the repository will have years to approach steady state; there will be ample solid material to nucleate and sorb actinides; and there is no thermodynamic driver for supersaturation. In addition, localized variation of the chemistry within the repository is not included in the model. As the brine flows through the repository through local variations in the chemistry, an "effective steady-state solubility" caused by dissolution, precipitation, and mixing is likely to occur. The concentration will change significantly from the predicted steady state only when the inventory of the actinide in the solid phase is depleted.

Extrapolation. It is not clear how accurate the models are when they are used for regions outside the conditions for which the parameters were obtained. Laboratory measurements were carried out over a range of pCO_2 conditions; however, extrapolation is required for some potential conditions within the repository. Use of MgO backfill eliminates the need to extrapolate to high pCO_2 and greatly simplifies the chemical conditions within the repository.

Confirmatory studies for the two brines at the $Mg(OH)_2$ - $MgCO_3$ buffer have been proposed by the AST group.

Oxidation State Analogy. The oxidation state analogy asserts that actinides in the same oxidation state have similar solubilities, although it has been observed that as the actinides increase in atomic number, each oxidation state shows the same general trends but with slightly decreasing solubility. The analogy is supported by pairs such as Am(+3) and Pu(+3), which show the same solubility. The analogy is not as clear cut, however, for the +4 oxidation state. Th(+4) appears to be somewhat more soluble than Pu(+4) and U(+4), so that use of Th(+4) as an analog is conservative.

WIPP Chemical Conditions. The uncertainty in the chemical conditions at the WIPP is harder to estimate. Experience shows that the most important chemical conditions within the repository include pH, f(CO2), major-ion concentrations in the brine, effective reducing power of the waste, and organic ligand concentrations.

Addition of excess MgO backfill greatly reduces the uncertainty in the pH and $f(CO_2)$. With relatively quick reaction times between CO_2 and MgO, the $f(CO_2)$ and pH are determined by the $MgCO3$ - $Mg(OH)2$ equilibrium within a given brine, so the uncertainty in pH and $f(CO_2)$ depend on the uncertainty of the major-ion concentrations in the brine.

EQ3/6 calculations have examined the chemical changes that may occur if Culebra brine were to enter the repository. If only Culebra brine enters the repository, it will dissolve the wall surface (93.2% halite, 1.7% each of polyhalite, gypsum, anhydrite, magnesite) until it is saturated with halite. The amount of the minor phases dissolved with the halite is not enough to cause saturation with these phases, and the resulting brine composition will be similar to Castile brine. If instead the brine circulates through the marker beds and disturbed rock zone where it may come into contact with more of the minor phases, it may saturate with all five minerals and have a composition close to that of Salado brine. Similarly, when Castile brine enters the repository, it may not change in composition appreciably unless it circulates through the marker beds and disturbed rock zone. There is considerable variation within each of these end-member brines, especially in the Mg concentration and the ionic strength (Brush, 1990). In addition, soluble salts such as $CaCl_2$ within the waste may change the major-ion concentrations within the brine at least locally. It is unlikely, however, that sufficient salts will be present to move the major-ion concentrations in the 20,000 to 30,000 m^3 of brine in the repository outside the range of concentrations defined by the Brine A and ERDA-6 end members. The AST predicted solubilities of the +3 and +5 oxidation states are within an order of magnitude of each other in these two brines, but the +4 oxidation state has a solubility more than two orders of magnitude lower in the Castile brine than in the Salado brine. Thus, if the mixed brines show actinide solubilities between the end-member brine solubilities, as expected for the +3 and +5 oxidation states, the uncertainty in the solubility due to uncertainty in brine composition is within the one-order-of-magnitude uncertainty estimated for the FMT predictions, but for the +4 oxidation state it is not. Thus the use of the Castile +4 solubility may underestimate the true solubility and use of the Salado +4 solubility may overestimate the true solubility.

The uncertainty in the effective reducing power of the waste results from the uncertainty in the kinetics of the redox reactions within the repository. Dilute ground waters are notorious for the disequilibrium between redox couples that is maintained for hundreds of thousands of years. The equilibrium between $S^=$ and $SO_4^=$, for example, is not established without the aid of microbes. Experiments and literature evaluation have revealed, however, that the more oxidized Am(+5), Np(+6), Pu(+5) and Pu(+6) species do not persist in WIPP conditions. The remaining uncertainty—U(+4) vs. U(+6), Pu(+3) vs. Pu(+4), and Np(+4) vs. Np(+5)—can result in large solubility differences. Because this issue is unresolved, the uncertainty has been handled by sampling on a single variable that gives the lower oxidation states 50% probability and the higher oxidation states 50% probability.

Uncertainty about the organic ligand concentrations is associated with four parameters:
- the amount of these ligands that will be emplaced with the waste;
- the rate at which microbes may digest them;
- the rate that microbes may generate new organic ligands; and
- the amount of water that may be required before release up a borehole is possible.

The greatest uncertainty comes from the first two of these. Some estimates of organic ligands come from records of how much of each was purchased by the waste generators and does not take into account the possibility that the ligands were destroyed during processing or disposed of in other waste streams (e.g., LLW, hazardous waste, sanitary waste, etc.). Other estimates were from waste generators who did not keep records when the amount was below a fairly high cutoff. The waste generator estimates (Watkins, 1996) are the only ones available; the Project has not tried to model this uncertainty. Weinar (1996b) calculated organic ligand concentrations by dissolving the BIR organic ligand inventories in 30,000 m^3 of brine; the resulting predicted FMT actinide concentrations were in most cases only slightly elevated above the solubility values predicted in the absence of the organic ligands. More-recent work has shown that there is no significant brine release up the borehole unless the repository is at least 50% saturated, which corresponds to a brine volume of about 20,000 m^3. Because the organic ligands increase the dissolved concentrations in the worst case by about an order of magnitude and have no effect on the colloid concentrations, the Project decided to use the solubility with the organic ligands in the PA.

7. FEPs Associated with Model Development

DR-13, Effects of chemical changes due to gas generation and corrosion
GG-7, Heat from exothermic reactions and concrete hydration
SP-7, Heat from concrete hydration
GG-4, Effect of thermal gradient
DR-15, Electrochemical effects
DR-16, Other second-order FEPs similar to electro-chemical effects
RNT-25, Electro-chemical effects in the repository
SP-5, Chemical degradation of seals
SP-8, Effects of microbial growth on concrete

8. History of Model Development and Alternatives Considered and Rejected

When work on the WIPP began in 1978, brine flow through the repository was not considered because none was expected. The 1985 promulgation of 40 CFR Part 191, the regulation that requires consideration of human intrusion (and thereby a flow of brine through the repository), mandated consideration of scenarios in which the repository would be humidified or inundated. These scenarios required investigation of potential mobilization of actinides, including actinide solubility in brine.

The solubility of actinides in the WIPP was initially estimated by an expert panel that reviewed the existing literature on actinide solubilities (Trauth et al., 1992). The range of solubilities obtained was about 14 orders of magnitude, because the chemical conditions surveyed included extremes of acidity and other conditions that may not occur in the inundated repository. The expert panel also estimated the effect of high carbonate concentrations (which are known to dramatically increase actinide solubility) on the actinide solubility despite the paucity of data for carbonate solutions. Median solubilities developed by the panel were Th, 10^{-10} M; U, $10^{-3.3}$ M; Np, 10^{-7} M; Pu, $10^{-9.2}$ M; and Am and Cm, 10^{-9} M (Trauth et al., 1992, p. 4-5). Published studies of actinides under conditions of relatively low solubility (i.e., neutral or basic pH) had focused on actinides in surface waters and ground waters that are considerably more dilute than WIPP brines. Modeling and experiments were therefore initiated to investigate actinide solubility in brines that simulated the composition of WIPP brine under conditions that might be expected to occur in the repository. These conditions include a pH range from about 4 to about 13, salt concentrations of the order of 5 M, and CO_2 overpressures (from microbial activity) up to lithostatic pressure.

Experimental investigations for other radioactive-waste projects (e.g., Nitsche, 1987) have approached the question of potential actinide solubility by measuring the solubility of the actinides in the waste directly. Although this is possible for well-characterized and homogeneous waste and ground waters, the waste intended for the WIPP is heterogeneous, and a wide range of chemical conditions are possible in the repository. Measuring solubility directly and ensuring that the measurements reflected steady-state WIPP conditions would entail an extremely large number of measurements and considerable uncertainty. The current approach of determining oxidation state distribution and modeling the solubility of each oxidation state was deemed preferable and more feasible.

Several thermodynamic models can be used to estimate activity coefficients and thus model solubilities. Four modeling approaches were considered: the Pitzer approach; the Harned's Rule approach, which uses ion pairing; a hybrid of the ion-pairing and Pitzer formalisms; and the specific ion interaction (SIT) ion-pairing approach. The Pitzer approach had been applied far more frequently to concentrated electrolyte solutions, so that a considerable literature using it has been developed (Novak, 1995). The Harned's Rule approach has been applied successfully to sea water and to dilute solutions, but not to salt solutions more concentrated than about two molal. Since the Harned's Rule approach offered no advantage of simplicity, it was rejected in favor of the Pitzer approach.

The SIT model is based on the assumption that only species with opposite charges interact, while the Pitzer approach includes interactions of neutral and like-charge species. SIT had been applied to simpler solutions of actinides in pure $NaClO_4$ or NaCl solution, but not successfully to complex brines. Moreover, SIT predictions of solubilities appeared to be reasonable only as high as about 3.5 molal. SIT was therefore also rejected in favor of the Pitzer approach. A Pitzer-SIT hybrid had been proposed for the lanthanides, but existing publications do not compare the calculated lanthanide solubilities with data, so the hybrid was rejected. Recent work by Janecky (1996) applies SIT to uranium in WIPP brines and appears to give results consistent with the Pitzer approach, which Janecky states are mainly useful for follow-on experimental design.

The HMW/FW parameterization of the Pitzer model was selected as the best formalism and primary concentrated-electrolyte data base for the AST dissolved concentration submodel. As noted in Section 3, HMW/FW provides an established data base for describing solubility behavior in the WIPP brine systems. Selecting the HMW/FW data base for the non-radioactive constituents in WIPP brines allowed the Project to concentrate on including the actinides of interest to the WIPP and the organic waste constituents that may affect dissolved actinide concentrations. Including the actinides in the model also necessitated reinterpretation of published actinide data to be consistent with the HMW/FW framework. These data were supplemented by a relatively small number of chemical measurements for the WIPP.

While FMT modeling of each of the actinides in all possible valence states with and without redox equilibrium would have been ideal, obtaining the appropriate parameters for all four possible valence states of plutonium, for example, would have entailed a complex and expensive experimental effort that was unrealistic. The strategy for the dissolved concentration model is therefore to group the actinides by oxidation state, because actinides in the same oxidation or valence state exhibit similar chemical behavior due to the similarities in their electronic structure. Analogous chemical behavior determined by electronic structure is a touchstone of chemical periodicity, and the oxidation state analogy has been confirmed for several lanthanides and actinides. Further detail supporting use of the oxidation state analogy is given in Section 9.

Oxidation state distribution of the actinides has been determined from extensive literature studies (Weiner, 1996b) and from experiments done under DOE contracts. Stable oxidation states of Am, Cm, Th, and Np were identified from the literature. The stability of the +6 oxidation state was studied under contracts with LANL and ANL-E. Uranium oxidation states were designated with reference to Grenthe et al. (1992).

9. Additional Information Supporting Model Choice and Confirmation

The Pitzer approach has been applied to high-ionic-strength systems (Pabalan and Pitzer, 1991; Novak, 1995, p. 25) and provided good correlation with experimental data. The approach yields solubilities of actinides in simulated WIPP brines that are generally within an order of magnitude of solubilities experimentally measured in similar systems (e.g., Novak and Roberts, 1994; Kim et al, 1985).

Under WIPP conditions Th, Am, and Cm exist in only one oxidation state. The aqueous solution chemistry of Cm is almost exclusively that of Cm(+3), and the analogy with Am(+3) has been extensively observed (Katz et al., 1986, v. 2, pp. 978 ff.). Analogous behavior between Pu(+3) and Am(+3) has also been observed in brines, although at lower pH values than are expected in the WIPP (Felmy et al., 1989). Pitzer parameters for the +5 state were developed for Np(+5), the only actinide expected to be present in the +5 state. The only actinide expected to be present in the +6 state is U(+6); its solubility in WIPP brines is being determined by empirical observations.

Th(+4) is the analog for U(+4), Np(+4), and Pu(+4), although the analogy as not as good as for the +3 oxidation state. The uncertainty in the use of Th(+4) is discussed in Section 6.

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10. Validity and Completeness Interface/Integration with PA and Computational Models

The dissolved actinide source term and the codes NUTS and PANEL all assume rapid approach to steady-state concentrations and uniform waste characteristics and inventory. Every effort has been made to integrate the results of BRAGFLO calculations with the calculations of the dissolved actinide source term. We have considered the rates of iron corrosion and microbial degradation of cellulosics in our consideration of the possible redox states of the actinides and the possible pH and f(CO$_2$). Both BRAGFLO and this conceptual model assume fast uptake of CO$_2$ by MgO and Mg(OH)$_2$. BRAGFLO brine volumes and flow rates were considered when calculating repository brine composition variation, and possible pH control by the CaCO$_3$-Ca(OH)$_2$ buffer. The effort was also coordinated with the colloid actinide source term, which assumes the same brines, f(CO$_2$), and pH. In addition, the humic and microbe colloid concentrations are determined using the uncomplexed actinide concentrations and proportionality constants. Caps on the total amount of actinides mobilized on microbes was also based on the total mobilized actinide, not just the colloid-mobilized actinide. Transport modeling in NUTS and PANEL will not include retardation due to chemical sorption, and molecular diffusion will

not be a significant factor, so the dissolved and colloidal actinides will be transported together to simplify modeling, except in the Culebra.

Transport in the Culebra, however, requires separate consideration of dissolved and colloidal actinides because retardation by both physical and chemical processes will be included. The total actinide concentration leaving the borehole and entering the Culebra will be repartitioned into dissolved and colloidal components prior to use by the SECOFL2D code, based on their relative concentrations in the repository. Because the redox state of the actinides leaving the repository is expected to be relatively unaffected by mixing with the Culebra waters and formation, the K_ds used in the Culebra will be based on the same redox states as the dissolved actinide source term and will use the same sampled parameter to determine those states. In addition, the assumed pmH and $f(CO_2)$ of the repository were considered when establishing the range of K_ds in the Culebra.

Colloidal Actinide
Source Term

1. Model Name

Colloidal Actinide Source Term

2. Responsible Contact

H. Papenguth

3. Model Description and References

Colloidal particles are of interest to the WIPP Project because they can provide a medium for the transport of actinides in flowing fluid. Colloidal particles are expected to form in the repository by several processes, including waste degradation, microbial activity, rock decomposition, and chemical condensation. They may also be carried into the repository by liquids moving from the Salado or through boreholes. Because of the presence of soils, nutrients, and cellulosic substrates for microbial action in WIPP waste (see Appendix BIR), humic substances and microbes will be present in disposal room brines.

Actinides in solution can bind to colloidal particles, primarily by sorption, and be carried with the particles. This is the principal way in which mineral fragments, humic substances, and microbes become carriers of colloidal actinides. Particles that behave as colloids may also form in the disposal rooms by condensation of dissolved actinides.

Four types of colloidal particles are believed to cover the range of possible behavior of all colloid types: microbes, humic and fulvic acids (humic substances), actinide-intrinsic (intrinsic), and mineral fragments. The concentration of actinides carried on each colloidal particle depends on many of the same chemical conditions that govern the concentration of dissolved actinides (see Sections 6.4.3.4 and 6.4.3.5).

The Project assumes that thermodynamic equilibrium is achieved for actinide concentrations contained by actinide-intrinsic and humic-type colloids. However, instead of using the principle of thermodynamic equilibrium for the concentration of actinides on mineral fragments and microbes, the Project adopts the conservative position that these particles, onto which actinides may sorb, are present in the aqueous phase in a constant quantity (steady-state). Moreover, rigorous equilibrium is not assumed between the dissolved phase and colloidal phase, which essentially produces two independent source terms.

For performance assessment, the concentration of each actinide element on each colloidal particle type during a realization is a fixed value. The concentration parameters are summarized in Table 6-9 and discussed in detail in Appendix PAR. Actual values of actinide concentration on colloidal particles are constrained by inventory limits.

Colloidal particles occur naturally in the Culebra, and dissolved actinides transported may sorb onto them; a conceptual model for these interactions is specified. Because the concentration of actinides in the Culebra must be less than the source concentration in the repository due to

dilution and other factors, the concentration of actinide-intrinsic colloids cannot increase in the Culebra. The DOE, however, assumes their concentration in the Culebra is the same as their concentration in the repository. The concentration of actinides on humic substances is a function of the concentration of dissolved species and is limited by the solubility of humic substances. Because humic substances will not be more soluble in the Culebra than in the repository, the concentration of actinides on humic substances cannot increase in the Culebra. Similarly, the concentration of actinides on microbes is a function of the concentration of dissolved species and is limited by the population of microbes. Because the population density of microbes in the Culebra is no greater than the repository population density, the steady-state assumption applied for microbes in the repository is appropriate for the Culebra as well. Mineral-fragment colloids in Culebra ground water, however, may sorb some actinides. It is expected that the concentration of mineral fragments in Culebra ground water will be small compared with the quantity of mineral-fragment colloids in the repository, and the total effect will be slight. To account for the potential increase, the DOE uses in performance assessment a source-term concentration of actinides carried by mineral-fragment colloids that is double the most reasonable repository concentration for this colloid type.

The concentrations of colloidal actinides determined by the conceptual model are assumed to be concentrations of mobile colloidal particles. The indicated concentrations will be entrained in moving brine. It is conservatively assumed that no actinides sorb onto colloidal particles that are not mobile in the repository. Thus all actinides in the repository will be present in the solid phase, dissolved in the aqueous phase, or as colloidal actinides suspended in the aqueous phase.

4. Model Purpose

The purpose of this model is to provide the source-term concentration of colloidal actinides in the repository for transport by fluid flow.

5. Principal Parameters and Relationship among Parameters Defined by the Model

The principal and only parameters in the conceptual model for the dissolved colloid source term are those that determine the concentration of various actinides on each colloidal particle. Consistent with the description of processes in the conceptual model, the concentration associated with actinide-intrinsic and mineral fragments are set constant at the upper end of a reasonable range determined from an experimental program. Also consistent with the conceptual model for the processes governing their concentrations, the actinide concentration on humic-type and microbial colloids is expressed as a proportionality of the aqueous concentration of the actinides of interest.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

In the event that the concentration of a particular dissolved actinide element (the sum of contributions of all of its possible oxidation states) and the concentration of that actinide associated with mobile colloidal particles together exceed the inventory-limited concentration of that actinide, actinide concentrations are distributed proportionally between dissolved and

colloidal phases. This approach was adopted because a conservative approach cannot be defined at this time.

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

The history of model development for the colloidal actinide source term is discussed in the section entitled, "Colloidal Actinide Transport in the Culebra."

9. Information Supporting Model Choice and Confirmation

In the repository environment, actinide solids present in the waste will dissolve according to thermodynamic principles until an equilibrium is established between the following entities:
- the actinide-bearing solid phase;
- dissolved actinide ions and complexes with anthropogenic organic ligands;
- actinide polyelectrolyte macromolecules (i.e., the immature actinide intrinsic colloid or polymer);
- actinides sorbed on fixed substrates (e.g., iron corrosion products);
- actinides sorbed onto immobile colloidal substrates; and
- actinides sorbed onto mobile colloidal sorbing substrates (e.g., humic substances).

Because of the complexities of evaluating the equilibrium relationships between these entities, the Project has elected to not take credit for sorption onto fixed substrates and to disregard the effects of competition associated with the equilibrium between dissolved actinides and actinides associated with colloidal particles. The concentration of actinides associated with mineral-fragment colloids is determined by bounding calculations, and so there is no equilibrium with the dissolved actinide concentration. The concentration of actinides associated with humic substances and microbes is linked to the dissolved actinide concentration by proportionality constants, which conservatively represent a very simple equilibrium relationship. In effect, the repository source term is reduced to two independent components that are only partially linked, resulting in an overestimate of the total concentration of mobile actinides that may leave the repository environment.

It is likely that the concentration of actinides sorbed on or contained within colloidal particles will be a function of various physicochemical conditions, such as pH, pCO_2, concentration of major brine constituents, ionic strength, oxidation speciation of the actinides, and concentration of organic ligands. Information on chemical conditions within the repository will be used to determine dissolved actinide concentrations and concentrations of actinides associated with the various colloidal particle types. The intrusion scenario selected for a particular PA realization will dictate the major-ion composition of the repository brine. In the event of an E1 or E1E2 intrusion scenario, the repository brine will be dominated by the brines introduced from the Castile Fm. because of the relatively high hydrostatic pressure in the Castile.

In an undisturbed scenario or an E2 intrusion scenario, the repository brine will consist of Salado Fm. brine. Key parameters associated with the intrusion scenario are calcium and magnesium concentration and ionic strength. The partial pressure of carbon dioxide and the pH may be controlled by the extent to which microbial degradation of wastes and corrosion of iron occurs in the repository or by backfill materials. The concentration of actinides associated with microbes could be linked to whether microbial gas generation is occurring; the Project has elected not to make that linkage, because lysed microbes may take part in actinide transport but not produce gas.

10. Validity and Completeness of Interface/Integration with PA and Computational Models

The mobile colloidal actinide source term depends partly on the dissolved actinide concentrations through proportionality constants (for microbes and humic substances).

Shafts and Shaft
Seals

1. Model Name

Conceptual model for long-term performance of the shafts and shaft seals.

2. Responsible Contacts

K. Knowles and F. Hansen.

3. Model Description and References

The four shafts connecting the repository to the surface are represented in performance assessment by a single shaft with a cross section and volume equal to the total cross section and volume of the four real shafts. The single, composite shaft is separated from the waste disposal regions in the model by the true north-south distance from the waste to the nearest shaft (the Waste Shaft). Upon closure of the repository, the shafts will be sealed as described in Section 3.3.2. The seal system is represented in performance assessment by nine materials occupying 11 model regions in the shaft: earthen fill from the surface to the Rustler Fm.; a clay region in the Rustler; asphalt at the top of the Salado; three concrete sections within the Salado; an upper clay region within the Salado; a thick section of compacted crushed salt; a lower clay section separated into upper and lower segments; and a concrete monolith at the repository horizon.

Conceptually, the shafts are assumed to be surrounded within the Salado by a disturbed rock zone (DRZ) with properties that vary with depth, time, and type of adjacent seal material. This DRZ is not represented explicitly in the BRAGFLO mesh. Rather, the mesh represents only the cross-sectional area of the shaft, and the permeability values for the various seal components at different times have been adjusted to account for the presence of the DRZ. This adjustment can be made because in Darcy flow the flux through a porous medium is a linear function of the product of the permeability of the medium and the cross-sectional area across which flow occurs. Thus, the flux that would occur through a shaft and its surrounding DRZ can be modeled equivalently using the shaft cross-sectional area with a higher permeability.

See also:

Section 6.4.4, Section 3.3.2, Appendix SEAL, Appendix SCR.2.3.8.2.

4. Model Purpose

The conceptual model for the shafts and shaft seals used in the performance assessment has been chosen to provide a reasonable and realistic basis for simulating long-term fluid flow through the shaft seal system and to allow evaluation of the effect that uncertainty about the long-term properties of the shaft seal system may have on cumulative radionuclide releases from the disposal system.

5. Principal Parameters and Relationships among Parameters Defined by the Model

Parameters used to characterize the shaft seal system are described in Section 6.4.4 and in Appendix PAR. The principal parameters of interest are the permeabilities and porosities of each seal component. For salt, concrete, and clay components, permeabilities are assumed to change with time. Permeabilities are constant for asphalt and earthen fill components. These parameters include the time-dependent properties of the DRZ around the shafts to determine the hydraulic properties of the shaft seal system through time. Other parameters specified for the BRAGFLO model include pore-volume compressibility, two-phase flow parameters, and initial conditions.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The conceptual model of the seals recommended to PA is based on results of detailed numerical models of the shaft seal system design. These models were developed to evaluate the performance of the shaft seal system under a range of conditions. Both fluid flow and structural response of the system have been evaluated. The principal uncertainties associated with the detailed models follow:

- reconsolidation of the crushed salt component;
- construction, permeability, and gas threshold pressure of the clay components; and
- damage, permeability, healing, and character of the Salado and Rustler disturbed rock zones.

These uncertainties are also present in the PA model. Seal parameters used by PA have incorporated these uncertainties (memorandum from M. K. Knowles to M. Tierney, January 17, 1996). The consequences of uncertainty in seal component performance were a primary motivation in the development of the proposed seal system design. Although there is uncertainty in many of the materials and models, the shaft will be completely filled with high density, low permeability materials. The use of multiple materials and components for each sealing function results in a robust system. Implementation of the seal system in the PA model ensures that calculational results will demonstrate the adequacy of the design. The proposed shaft seal system no longer makes a distinction between "short-term" and "long-term" seal components. Time dependency is incorporated directly into the model through temporal variation in seal properties.

7. FEPs Associated with Model Development

SP-1, Mechanical Effect of Gas Generation.
SP-2, WIPP Shaft Seal Degradation.
SP-3
SP-4, Other Physical Degradation Mechanisms (Cracking Concrete, Erosion of Seals).
SP-5, Chemical Degradation of Seals (Alkali-Aggregate, Cement Sulfate, Cement Pore Water).
SP-6, Differing Thermal Expansion.
SP-7, Concrete Hydration.
SP-8, Effects of Microbial Growth on Concrete.
SP-9, Effect on Groundwater Chemistry.

SP-10, WIPP Investigation Boreholes.
SP-11, Evaluation of Full Shaft Conceptual Model Seal System.

8. History of Model Development and Alternatives Considered and Rejected

The four shafts into the repository will be sealed after completion of disposal activities at the WIPP. The shaft seal system design has evolved over time (Stormont, 1988; Nowak, et. al., 1992; DOE 1995). The Initial Reference Seal System Design proposed a two-phase sealing strategy: short-term concrete and clay seals and a long-term crushed salt seal. The use of native rock (i.e., crushed salt) as a permanent sealing material is considered the most effective means to eliminate the shafts as a preferred pathway for migration of hazardous constituents. Due to the time necessary for the crushed salt to reconsolidate to sufficiently low densities, short-term seals were proposed as a means to prevent fluid migration during the interim. Estimates of this interim period ranged from 100 to 200 years.

Seal design changes and refinements have been incorporated into the conceptual model of the seals used by WIPP PA (WIPP Performance Assessment Department, 1990, 1991, 1992). Performance assessments conducted prior to 1992 addressed general sealing issues but did not include specific seal components. A baseline conceptual model and associated parameters for the shaft seal system is included in the July update to the Draft Compliance Certification Application (DOE/CAO, July 1995, Section 6.4.4). A discussion of the conceptual model for the shafts may also be found in the Baseline Position Paper for the Repository Seals Program (Section 4.0). This document also recommended changes in the seal conceptual model.

Results of the scoping calculations using the DCCA model demonstrated that low-permeability materials were required for the shaft seals (DOE/1995, Appendix D). However, the simplicity of the conceptual model limited the applicability of results to the detailed seal system design. A comparison of the scoping calculations to the seal system design proposed for the Compliance Certification Application may be found in a memorandum to PA (M.K. Knowles, June 29, 1995).

The current conceptual model of the WIPP shaft seals is documented in a memorandum to PA (M.K. Knowles, September 29, 1995). This conceptual model is easily related to the detailed seal design both visually and technically, since all materials and components of the engineered seals are included. Parameters for the materials were developed from field and laboratory testing, literature searches, and numerical modeling. The parameter development process will be published as a SAND document. Documentation on the process was included in the package submitted to PA in January, 1996.

References:

Stormont, J.C. 1988. *Preliminary Seal Design Evaluation for the Waste Isolation Pilot Plant.* SAND87-3083. Albuquerque, NM: Sandia National Laboratories.

Nowak, E.J., J.R. Tillerson, T.M. Torres. 1992. *Initial Reference Seal Design: Waste Isolation Pilot Plant.* SAND-90-0355. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1990. *Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1990.* SAND90-2347. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992. *Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1991.* SAND91-0893/3. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992. *Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1992.* SAND92-0700. Albuquerque, NM: Sandia National Laboratories.

Systems Prioritization Method - Iteration 2 Baseline Position Paper: Repository Seals Program.

Seal System Design Report; 1995. DOE/WIPP 95-3117. October 1995.

9. Information Supporting Model Choice and Confirmation

The processes that can affect the performance of the shaft seals are discussed in some detail in Appendices C and D of the Compliance Submittal Design Report (CSDR), to be published in August, 1996. Structural, hydrologic, and coupled structural/hydrological processes are considered in the CSDR. Evaluation of these issues required the use of existing structural and both single- and two-phase flow codes. In addition, development of conceptual and numerical models for crushed salt reconsolidation, the disturbed rock zone, and the shaft seal system was required. These models have been reviewed by independent, qualified experts, are well documented, and have been developed within an accepted QA program. Codes used in the analyses include SPECTROM-32 (structural), SWIFT II (single-phase flow), and TOUGH28W (multi-phase flow). These codes were selected for their capability to simulate the processes thought to affect seal performance. They are also well-documented, accepted, and widely used within the scientific community. The codes were modified to implement the conceptual models specific to the seals. These modifications were made within a software QA program.

Although it is possible to explore alternative models, codes, and methods, the purpose of the QA program is to assure the credibility of those have been used for the CCA.

10. Validity and Completeness Interface/Integration with PA and Computational Models

The BRAGFLO model of the seal system requires consistency with parameters associated with the surrounding system. For example, the permeability of the crushed salt component should always be greater than or equal to that of the intact halite. Similarly, the calculation of the effective halite DRZ permeability requires the permeability of intact halite as input. These

integration issues are well known by PA, and the processes necessary to address them were included in the delivery of the seal parameters to PA.

As noted in Section 9, there are parameters which result from coupled structural/hydrological processes. The seal parameters reflect this coupling.

The Salado

1. Model Name

The Salado (fluid flow)

2. Responsible Contacts

S. Howarth and R. Beauheim
P. Davies, A. Lappin, T. Christian-Frear

3. Model Description and References

The Salado Fm. is considered to be the principle natural barrier between waste and the accessible environment because fluid transport in intact Salado rock is slow due to the low permeability of the salt. In addition, because of the native high pressures of fluids there, even high pressures in the repository can create only modest hydraulic potential gradients in the Salado over the scale of the disposal system. Thus, the pathway of lateral transport in intact Salado is modeled, but it is considered unlikely to result in any significant radionuclide transport to the accessible environment boundary.

Fluid flow in the Salado is considered in the conceptual model of long-term disposal system performance for reasons other than the possibility of release through it under intact conditions. First, some liquid could move from the Salado to the repository due to the considerable gradients that can form for liquid flow inward to the repository. This possibility is important because such fluid can interact with creep closure, gas generation, actinide solubility, and other processes occurring in the repository. Second, gas generated in the repository is thought to be capable of fracturing the Salado interbeds under certain conditions, creating increased permeability channels that could be pathways for lateral transport. Fluid flow between the repository and Salado is the subject of this conceptual model; the fracturing conceptual model is developed separately.

The fundamental principle in the conceptual model for fluid flow in the Salado is that it is a porous medium within which gas and brine can both be present and mobile (two-phase flow), governed by conservation of energy and mass, and by Darcy's Law for their fluxes. Consistent with typical concepts of two-phase flow, each phase can affect the other by impeding flow due to partial saturation (relative permeability effects) and by affecting pressure by capillary forces (capillary pressure effects). It is assumed that no waste-generated gas is present initially, but gas can enter the interbeds. It is expected that the low permeability of impure and pure halite intervals of the Salado will prevent gas from penetrating due to the expected high capillary pressure for these units. Section 2.2 discusses the alternatives that have been seriously considered by the DOE for flow in the Salado.

There is some variability in composition between different horizons of the Salado. The largest differences occur between the anhydrite-rich layers called interbeds and those dominated by halite. Within horizons dominated by halite, composition varies from nearly pure halite to halite plus several percent other minerals, in some instances including clay (see Section 2.1). It

is thought that all of the Salado behaves as impure halite except those interbeds that intersect the DRZ near the repository. This conceptual model has been satisfactorily compared to an alternative model that explicitly represented all stratigraphically distinct layers of the Salado near the repository (Christian-Frear and Webb, 1996).

From other modeling and theoretical considerations, flow between the Salado and the repository is expected to occur primarily through interbeds that intersect the DRZ. Because of the large surface areas between the interbeds and surrounding halite, the interbeds serve as conduits for the flow of brine in two directions: from halite to interbeds to the repository, or, for brine flowing out of the repository, from the repository into interbeds and then into halite. Because of the effect of gravity in the relatively porous and permeable repository, brine is considered most likely (but not constrained) to leave the repository through Marker Bed 139 below the repository. Gas is considered most likely (but not constrained) to leave the repository through anhydrite interbeds above the repository.

The effect of gravity may also be important in the Salado due to the slight and variable natural stratigraphic dip. For long-term performance modeling, the dip in the Salado is taken to be constant and 1° from the north to south.

Fluid flow in the Salado is conceptualized as occurring either convergently upon the repository, or divergently from it, as discussed in detail in Section 6.4.2.1. Because the repository is not conceptualized as homogeneous, implementing the conceptual model of convergent or divergent flow in the Salado is somewhat complicated and is discussed in Section 6.4.2.1.

4. Model Purpose

The purpose of this model is to reasonably represent the effects of possible fluid flow in the Salado on long-term performance of the disposal system.

5. Principal Parameters and Relationship among Parameters Defined by the Model

The concept of Darcy flow for two phases implies certain important parameters. Some principal parameters relate to the properties of the fluid, others to the rock. Fluid properties in the Darcy flow model used for WIPP are its density, viscosity, and compressibility. Rock properties in Darcy flow models are porosity, permeability, and pore compressibility. Other parameters are required to describe the interactions or interference between the two phases present in the model, gas and brine, because they can occupy the same pore space. In the WIPP application of these models, compressibility of both the liquid and rock are related to porosity through a dependence on pressure. Fluid density, viscosity, and compressibility are often closely related to fluid composition, pressure, and temperature. For the WIPP, fluid

viscosity is a function of pressure, but its density and compressibility are held constant. Fluid composition for the purposes of modeling flow and transport is assumed to be constant.

The conceptual model for Salado fluid flow has primary interactions with three other conceptual models. The interbed fracture conceptual model allows porosity and permeability of the interbeds to increase as a function of pressure. The repository fluid flow model is directly coupled to the Salado fluid flow model by the governing equations of flow in BRAGFLO (in the governing equations of the mathematical model, they cannot be distinguished), and it differs only in the region modeled and the parameters assigned to materials. The Salado model for actinide transport is directly coupled to the conceptual model for flow in the Salado through the process of advection.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

All sensitivity calculations done to date assume both a flat-lying repository and adequacy of the radial-flow approximation. Sensitivity analyses performed as part of the 1992 preliminary PA identified the relative importance of sampled parameters with respect to human-intrusion scenarios and undisturbed performance. For human intrusion, parameters were ranked as follows (WIPP Performance Assessment Department, 1993, p. 9-8):
- two parameters were considered critically important, neither is a Salado parameter;
- five parameters were considered very important; including Salado halite permeability #1, Salado anhydrite permeability #2;
- two parameters were considered important; neither is a Salado parameter;
- twenty-four parameters were considered less important; six were Salado parameters (listed alphabetically): Residual brine saturation, Brooks-Corey model exponent; Brooks-Corey, van Genutchen pointer; Brooks-Corey residual gas saturation; Salado anhydrite porosity; far-field pressure in Salado.

For undisturbed performance, parameters were ranked as follows (WIPP Performance Assessment Department, 1993, p. 9-8):
- six parameters were considered very important, including from the Salado the #2 anhydrite permeability;
- eleven parameters were considered important, including four from the Salado (listed alphabetically): Brooks-Corey, Van Genutchen pointer; Salado anhydrite porosity; Salado halite permeability;
- eight parameters were considered less important, including four from the Salado (listed alphabetically): residual brine saturation; Brooks-Corey model exponent; residual gas saturation; far-field pressure.

References:

WIPP Performance Assessment Department. 1993. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992, Volume 4: Uncertainty and Sensitivity*

Analyses for 40 CFR 191, Subpart B, Section 4.1, Model Geometry, pp. 4-1, 4-3, SAND92-0700/4.

7. FEPs Associated with Model Development

See Section 9.

8. History of Model Development and Alternatives Considered and Rejected

In the 1980 FEIS (Table 1-1, pg. 1-7 - 1-8, Lappin et al., 1989), the Salado Fm. was assumed to be a confining bed, containing no circulating ground water (p. 7-87). Brine was thought to be present only in fluid inclusions and hydrous minerals. Brine was assumed not be present along grain boundaries. Gas permeability was estimated to be adequate to dissipate the volumes of gas potentially generated by the waste. There was no explicit recognition of any differing hydrologic role for the non-halite interbeds.

Based on the results of early *in situ* testing, the conceptual model of the Salado Fm. had changed by the time of publication of the DSEIS (Table 1-1, pg. 1-7 - 1-8, Lappin et al., 1989). Grain boundary brines were known to be present and distinct compositionally from fluid inclusions. The Salado was interpreted to be hydrologically saturated. The major contribution to fluid flow was interpreted to be movement of grain-boundary fluids, as a result of pore pressure gradients resulting from excavation. Darcy flow, assuming atmospheric boundary conditions within the repository (which was all that could be modeled at the time), probably over-predicted brine inflow. Far-field permeability (not distinguished between halites and anhydrites) was thought to be less than 10^{-21} to 10^{-22} m^2 and possibly even effectively zero in undisturbed regions, based on limited in-situ tests. Because gas would have to displace brines in the country rock, dissipation of significant volumes of gas would be difficult. The combination of gas-generation rates and low permeability would have led to pressures exceeding lithostatic unless these pressures were relieved: numerical models for altered anhydrites did not exist at that time. Except at seal locations, MB 139 was thought to be a relatively high-permeability path directly under the excavations because of the development of open excavation-related fractures.

In a performance assessment completed in December 1992 (WIPP Performance Assessment Department, 1992, pp. 2-41—2-45), anhydrite interbeds provided the dominant pathway for fluid migration because of their relatively high permeability. New far-field test data indicated permeabilities of 10^{-16} to 10^{-21} m^2 for anhydrites and 10^{-20} to 10^{-24} for halite. (The Project interpreted the low ends of these ranges to be "far-field" permeabilities and the higher ends to results from excavation effects; pp. 2-55, 2-56). It was newly recognized that there would be coupling between fluid flow, creep closure, and brine-dependent gas generation. No altered-anhydrite model was implemented in the performance assessment.

In 1994, the Project concluded that the regional one-degree stratigraphic dip would likely have a significant effect on fluid flow into and out of the repository. An altered-anhydrite model for interbed fracture under elevated gas pressures was implemented. Flow simulations incorporating detailed stratigraphy confirmed that simplifications considering only a "lumped" impure halite were adequate. The potential for preferential brine outflow due to channeling, fingering, up-dip flow, or fracturing was also recognized and considered important. Uncertainty about the adequacy of the 2D modeling simplification to provide reasonable estimates of three-dimensional brine inflow and outflow was thought to be potentially important, because of addition of both dip and altered-anhydrite "fracturing" model.

In 1995, final analysis of the Room Q experiment showed experimental results to be consistent with Darcy flow model.

References:

Lappin, A.R., R.L. Hunter, D.P. Garber and P.B. Davies, ed. 1989. *Systems Analysis, Long-Term Radionuclide Transport, and Dose Assessments, Waste Isolation Pilot Plant (WIPP), Southeastern New Mexico; March 1989.* SAND89-0462. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 2: Technical Basis.* SAND92-0700/2. Albuquerque, NM: Sandia National Laboratories.

9. Information Supporting Model Choice and Confirmation

S-1: Verification of 2D radial flaring using 3D geometry. It was concluded that the 2D flaring approach is adequate for brine inflow and outflow.

S-3: One degree dip: Concluded that CCA calculation should include one-degree dip screened into calculations.

S-4 (mechanical effects of gas generation) and S-5 (brine storage in anhydrite and halite): "Pressurization induced by the generation of gases may effect the mechanical properties if anhydrites in the Salado (S4)...changes in mechanical properties will affect brine storage in anhydrite (S5)."

Radial brine outflow was implemented in the CCA model, based directly on CCA text (section 6.4.5.4) arguing that preferential flow mechanisms will be negligible.

1. Model Name

Anhydrite Interbed Fracture Model

2. Responsible Contact

Palmer Vaughn

3. Model Description and References

It is expected that the pressure in the repository cannot greatly exceed lithostatic because the rock would fracture if subjected to higher stresses. Fractures create void volume and may allow fluids more rapid access to other pore volume, both of which counteract pressure buildup. It is thought that the anhydrite interbeds that intersect the DRZ will have their porosity and permeability altered if pressure rises to within about one MPa of lithostatic pressure. Porosity and permeability are expected to be altered only in the anhydrite interbeds because they contain natural fractures in most locations, some of which contain infilling minerals. These structural weaknesses are more prone to dilation or new fracturing than halite-rich horizons of the Salado, which do not contain fractures.

The porosity and permeability increases are conceptualized as occurring throughout the affected interbed; in other words, throughout the porous medium as a whole rather than on discrete portions. This simplification facilitates numerical implementation and execution.

4. Model Purpose

The purpose of this model is to alter the porosity and permeability of the anhydrite interbeds if their pressure approaches lithostatic, simulating some of the effects of fractures with the intent that unrealistically high pressures do not occur in the repository or disposal system.

5. Principal Parameters and Relationships among Parameters Defined by the Model

Two parametric behaviors must be quantified in the conceptual model. First, the change of porosity with pressure in the anhydrite marker beds must be specified. This is done with a relatively simple equation, described in Appendix BRAGFLO, that relates porosity change to pressure change using an assumption that the fracturing can be thought of as increasing the compressibility of interbeds. Parameters in the model are treated as fitting parameters and have little relation to physical behavior except that they affect the porosity change. The second parametric behavior is the change of permeability with pressure, which is incorporated by a functional dependence on the porosity change. It is assumed that a power function is appropriate for relating the magnitude of permeability increase to the magnitude of porosity increase. The parameter in this power function, an exponent, is also treated as a fitting parameter and can be set so that the behavior of permeability increase with porosity increase fits the desired behavior.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The fracture enhancement model assumes fracture propagation is uniform in the lateral direction to flow within the marker beds. That is, within the accuracy of the finite difference grid, a fracture will develop radially outward. This would not account for fracture fingering or a preferential fracturing direction; however, no existing evidence supports heterogeneous anhydrite properties that would contribute to preferential fracture propagation.

The maximum enhanced fracture porosity controls the storativity within the fracture. The extent of the migration of the gas front into the marker bed is sensitive to this storativity. The additional storativity due to porosity enhancement will mitigate gas migration within the marker bed. The enhancement of permeability by marker-bed fracturing will make the gas more mobile and will contribute to longer gas-migration distances. Thus the dual effects of porosity and permeability enhancement are tradeoffs in affecting the gas-migration distances.

Since intact anhydrite is partially fractured (Key et al., 1994), the pressure at which porosity or permeability changes are initiated is close to the initial pressure within the anhydrite. The fracture initiation pressure is assigned a value of 0.2 MPa above the initial brine pressure.

The fracture treatment within the marker beds will not contribute to early brine drainage from the marker bed, since the pressures at these times are below the fracture initiation pressure.

7. FEPs Associated with Model Development

FEP S-1, Dynamic Alteration of the DRZ/Transition Zone. This FEP considers the effect of fracturing within the Salado DRZ. This is discussed in the Salado DRZ write-up.

8. History of Model Development and Alternatives Considered and Rejected

In the 1992 PA analysis, repository pressures were shown to greatly exceed lithostatic pressure (approximately 14.7 MPa) when high gas generation was achieved. Pressures within the waste repository and surrounding regions were roughly 20 to 25 MPa. It was expected that fracturing within the anhydrite marker beds would occur at pressures slightly below lithostatic pressure. An expert panel on fractures was convened to develop the conceptual bases for the fracturing within the anhydrite marker beds (Key et al., 1994).

9. Information Supporting Model Choice and Confirmation

The input data that control anhydrite fracturing were chosen deterministically to produce the appropriate pressure response as predicted by the linear elastic fracture mechanics model (LEFM). Preliminary results from the current CCA calculations show that repository pressures do not exceed the full fracture pressure of approximately 16.5 MPa, a value slightly higher than lithostatic pressure.

10. Validity and Completeness Interface/Integration with PA and Computational Models

The computational results have been tested numerically and the model has been integrated into the BRAGFLO code.

References:

Key, S., et.al. 1994. *Background and Basis for the Fluid Flow Model Incorporated in BRAGFLO for Representing Pore Pressure-Induced Alterations in Permeability and Porosity in the Anhydrite Interdbed Above and Below the WIPP Repository Horizon.* SAND94-0381. Albuquerque, NM: Sandia National Laboratories.

Fluid Flow in the
Salado DRZ

1. Model Name

Conceptual model for long-term fluid flow in the disturbed rock zone (DRZ) within the Salado Fm. around the waste disposal, operations, and experimental regions.

2. Responsible Contact

P. Vaughn.

3. Model Description and References

As discussed in Chapter 3, permeability and porosity in the DRZ near the repository are expected to generally increase as a result of a variety of processes, including creep closure and stress-field alterations. The increase in DRZ permeability increases the ability of fluid to flow between anhydrite interbeds and the waste disposal region. The increase in DRZ porosity provides a volume in which some fluid could be retained so that it does not contact waste or so that it slows actinide movement. Performance assessment approximates the effects of the DRZ conservatively with respect to brine flow to the repository. The permeability of this region is increased relative to intact Salado rock for the duration of a realization, in part because the increases in permeability and porosity in anhydrite interbeds are not expected to be completely reversible with creep closure of the disposal rooms. The porosity of the DRZ is assumed to be small to reduce fluid retention in the DRZ. The DRZ extends above and below the repository from the base of MB 138 to the base of MB 139. The performance assessment treatment of the DRZ creates a permanent high-permeability region that does not significantly impede flow between the repository and affected interbeds.

See also:

Section 6.4.5.3, Section 3.3.1.1, Appendix SCR Section SCR.2.3.1

4. Model Purpose

The conceptual model for the DRZ around the waste disposal, operations, and experimental regions has been chosen to provide a reasonably conservative estimate of fluid flow between the repository and the intact halite and anhydrite marker beds.

5. Principal Parameters and Relationships among Parameters Defined by the Model

Parameters used in the conceptual model for the DRZ are described in Section 6.4.5.3 and Appendix PAR. The principal parameters of interest are permeability and porosity, which have the largest effects on fluid flow. Other parameters specified for the BRAGFLO model include rock compressibility and two-phase flow parameters.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Because the model does not use sampled parameters to characterize uncertainty about the properties of the DRZ, it does not allow evaluation of the effect of the DRZ on uncertainty in cumulative radionuclide releases from the disposal system. Instead, the approach taken conservatively estimates any contribution the DRZ might make to the long-term performance of the natural barriers.

7. FEPs Associated with Model Development

S-6.

See also:

Records package entitled "FEPs Screening Analysis for FEPs DR2, DR3, DR6, DR7, and S6."

8. History of Model Development and Alternatives Considered and Rejected

The Salado DRZ extends above and below the repository from the base of MB 138 to MB 139. This zone provides a high-permeability region that does not significantly impede flow between the repository and interbeds. The permeability and porosity increases in this region are predominantly due to creep closure, possible room expansion, and fracturing caused by high pressures. Performance assessment approximates the DRZ properties with a constant low porosity equal to those of the intact halite units and a constant high formation permeability. This conservative combination of properties will enhance fluid flow in the DRZ and decrease fluid storage.

A screening analysis examined the effect of dynamic alteration of permeability and porosity properties in the DRZ to determine whether constant DRZ properties are conservative with respect to brine and gas outflow. This analysis implemented a fracturing model in BRAGFLO for the DRZ. This fracturing model is identical to the existing anhydrite interbed alteration model. In this model, formation permeability and porosity depend on brine pressure as described by Key et al. (1994). This model permits the representation of two important formation alteration effects. First, pressure build-up due to gas generation and creep closure within the waste will slightly increase porosity within the DRZ and offer additional fluid storage with lower pressures. Second, the accompanying increase in formation permeability will enhance fluid flow away from the DRZ. Since an increase in porosity tends to reduce outflow into the far field, parameter values for this analysis were selected so that the DRZ/TZ alteration model greatly increases permeability while only modestly increasing porosity.

Two basic scenarios were considered in the screening analysis, undisturbed performance and disturbed performance. Both scenarios included a 1-degree formation dip downward to the south. Intrusion event E1 is considered in the disturbed scenario and consists of a borehole that penetrates the repository and pressurized brine in the underlying Castile Formation. Two variations of intrusion event E1 are examined, E1 Up-Dip and E1 Down-Dip. In the E1 Up-Dip event, the

intruded panel region is located on the up-dip (north) end of the repository, whereas in the E1 Down-Dip event, the intruded panel region is located on the down-dip (south) end of the repository. These two E1 events permitted evaluation of the possibility of increased brine flow into the panel region due to higher brine saturations down-dip from the borehole and the potential for subsequent impacts on contaminant migration. To incorporate the effects of uncertainty in each case (E1 Up-Dip, E1 Down-Dip, and undisturbed), a Latin hypercube sample size of 20 was used, for a total of sixty simulations. To assess the sensitivity of system performance on formation alteration of the DRZ and TZ, complementary cumulative distribution functions (CCDFs) of normalized contaminated brine releases to the Culebra after human intrusion via the shaft system, as well as releases to the subsurface boundary of the accessible environment, were constructed and compared with the corresponding baseline model CCDFs that were computed with constant DRZ permeability and porosity values. Based on comparisons between CCDFs, computed releases to the accessible environment were determined to be essentially equivalent between the two treatments.

Reference:

Key, S., et.al. 1994. *Background and Basis for the Fluid Flow Model Incorporated in BRAGFLO for Representing Pore Pressure-Induced Alterations in Permeability and Porosity in the Anhydrite Interdbed Above and Below the WIPP Repository Horizon,* SAND94-0381. Albuquerque, NM: Sandia National Laboratories.

See also:

FEPs Screening Analyses, Records Package, SWCF:1.1.6.3:PA:NG:TSK:DR2,DR3,DR6,DR7, and S6

9. Information Supporting Model Choice and Confirmation

See Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See Section 8.

1. Model Name

Actinide Transport in the Salado

2. Responsible Contacts

P. Vaughn

3. Model Description and References

Actinide transport in the Salado Fm. is conceptualized as occurring only by advection through the porous medium described in the Salado hydrology conceptual model. Advection is the movement of material with the bulk flow of fluid. Other processes that might disperse actinides, such as diffusion, hydrodynamic dispersion, and channeling in discrete fractures, are not included in the conceptual model.

4. Model Purpose

The purpose of this model is to represent the transport of actinides in the Salado.

5. Principal Parameters and Relationship among Parameters Defined by Model

Advection is a direct function of fluid flow, which is discussed in the conceptual model for Salado fluid flow.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

NUTS treats the transport of five carefully-selected "lumped" radioisotopes within all the regions for which BRAGFLO computes brine and gas flow. The brine must pass through some part of the repository at some period in its history to be of interest. While there, it acquires radioisotopic constituents, which it then transports by various means to other regions outside the repository. NUTS uses BRAGFLO's velocity field, pressures, porosities, saturations, and other model parameters (including geometrical grid, residual saturation, material map, brine compressibility, and time step) averaged over a given number of time steps (20 for the CCA calculation), which it takes as input for its transport calculations. Consequently, NUT's results are subject to all the uncertainties associated with BRAGFLO's conceptual model and parameterization, which will not be repeated here.

The five radioisotopes treated by NUTS are lumped in two different ways. First, for decay purposes, similar radioisotopes having similar half lives are lumped and given the longest half life of the group. Second, for transport purposes, lumped solubilities represent both dissolution and colloidal formation. Lumping introduces uncertainty, but it should be conservative. In return, lumping simplifies and expedites numerical aspects of the computations, reducing the burden on machine time. If calculated releases based on lumped isotopes approach EPA limits, the limiting cases may be recalculated using actual radioisotopic data. Lumping is based on the

nineteen radioisotopes having potential EPA normalized releases greater than 0.01. Details of the lumping are discussed in the sections on actinide source terms.

NUTS disregards sorptive and other retarding effects throughout the entire flow region, even though retardation must occur at some level within the repository, the marker beds, and the anhydrite interbeds, and especially in zones with clay layers or clay as accessory minerals. Disregarding retardation introduces a conservative bias into NUT's predicted results.

Because the time scale for assessment is measured in millennia, NUTS ignores reaction-rate aspects of dissolution and colloid chemical processes. Dissolution and precipitation are assumed to take place instantaneously, which affords great computational ease and is conservative.

NUTS neglects molecular dispersion, which leads to uncertainty. For materials of interest in the WIPP repository system, molecular diffusion coefficients are at a maximum on the order of 4×10^{-10} m^2/s. Thus, the simplest scaling argument using a time scale of 10,000 yrs leads to a molecular diffusion (i.e., mixing) length scale of ~10 m, which is negligible compared to the lateral advection length scale of roughly 2,400 m (the distance from the repository to the edge of the land withdrawal boundary).

NUTS also neglects mechanical dispersion, which leads to additional uncertainty. Mechanical dispersivities are empirical (tensor) factors that are proportional to flow velocity (to within geometrical factors related to flow direction). They account for both the downstream and cross-stream spreading of local extreme values in concentration of dissolved constituents. Physically, the spreading is due to the fact that both the particle paths and velocity histories of once-neighboring particles can be vastly different due to material heterogenieties characterized by permeability variations. These variations arise from the irregular cross-sectional areas and tortuous nonhomogeneous, nonisotropic connectivity between pores that occur in WIPP (and other natural) mineral deposits. Because of its velocity dependence, the transverse component of mechanical dispersivity tends to transport dissolved constituents from regions of high flow (where mechanical dispersivities are largest) to regions of slower flow (where dispersivities are smaller). In the downstream direction, dispersivity merely spreads constituents in the flow direction. Ignoring lateral spreading assures that dissolved constituents will remain in the rapid part of the flow field, which assures their transport toward the boundary. Ignoring longitudinal dispersivity ignores the elongation of a feature in the flow direction, which ignores foreshortening (or lengthening) of arrival times. However, because the EPA release limits are time-integrated measures, the exact times of arrival are unimportant, so long as a constituent arrives at the land withdrawal boundary within the assessment period (10,000 yr). Ignoring mechanical dispersivity is therefore conservative.

Advection is therefore the principal NUTS transport mechanism, which underscores NUT's reliance on BRAGFLO. Because the Darcy flows are given to NUTS as input, the maximum solubility limits for combined dissolved and colloidal components are the most important NUTS parameters. They are described in the section on actinide source terms.

The next most important transport mechanism after advection is decay, which can act as either a source or a sink. If radioisotopes are treated individually, the decay calculations performed by NUTS are without significant uncertainty. However, NUTS will not, as a rule, treat individual radioisotopes. Rather, in first-round computations, five "lumped" (or equivalent) radioisotopes will be considered, and that substitution will introduce limited uncertainty along with computational ease. The uncertainty in question is removable by recalculation using actual decay chains in all instances in which calculated releases approach EPA limits.

Because NUTS relies on BRAGFLO for input, any uncertainties that result from numerical concepts that apply to BRAGFLO carry over and apply also to NUTS. NUTS also introduces additional numerical uncertainties resulting from the applied numerical schemes.

7. FEPs Associated with Model Development

NUTS served in the evaluation of BRAGFLO's FEPs by converting BRAGFLO's flow measures to normalized releases. Thus, by association, NUTS played a role in BRAGFLO's FEPs.

8. History of Model Development and Alternatives Considered and Rejected

NUTS was originally conceived as a relatively straightforward approach to classical fluid transport, but an approach that had the capacity to treat virtually all special effects of interest in the study of radioactive migration. In a way, NUTS's analysts aimed intentionally toward an extremely inclusive design. However, FEPs studies and earlier system prioritization exercises suggested that a simplified version of NUTS was preferable in that results generated by the simplified model were sufficiently representative while run time was minimized. Thus, in arriving at the present model, many of NUTS's original design features were stripped away (see, for example, the NUTS User's Manual). NUTS's principal design features in its present form are, first, its ability to treat only the wastes that are actually encountered along the given flow path, which leads to a more realistic estimate of the fraction of the inventory that is available to the flow compared to other estimates, and second, its ability to trace downstream fluid and determine the fraction that actually contacted wastes.

9. Information Supporting Model Choice and Confirmation

Little latitude for choice is available in the way the NUTS code is written. Once conceptual aspects of the physical and chemical mechanisms to be modeled are decided (see Sections 6 and 7, above), it remains only to write the partial differential equations (Bear, 1988; Bear, 1993, Kazemi et al., 1976) that govern the processes, which is straightforward, and to devise means to integrate them numerically, which is also a relatively straightforward, although the coarseness of some grid blocks and time steps has stimulated debate. NUTS's grid is taken identically from BRAGFLO. The physical and chemical mechanisms involved in NUTS transports are well known and well studied. Model confirmation was established through comparison testing with other numerical models and known analytical solutions.

References:

Bear, J. 1988. *Dynamic of Fluids in Porous Media*. Dover Publications, Inc., NY.

Bear, J. 1993. *Flow and Contaminant Transport in Fractured Rock*. Academic Press, Inc.

Kazemi, H., L.S. Merrill, K.L. Porterfield and P.R. Zeman. 1976. *Numerical Simulation of Water-Oil Flow in Naturally Fractured Reservoirs*. SPEJ 317-326.

10. Validity and Completeness/Integration with PA and Computational Models

NUTS's interface with BRAGFLO is essentially perfect in completeness and validity in that NUTS takes virtually all its flow and flow-related attribute and property data from BRAGFLO and treats them as incontestable. Thus, the upstream interface is perfectly smooth.

NUTS computes transports throughout the entire BRAGFLO computational region, which includes the shaft and any intrusive boreholes that may occur, the marker beds, the anhydrite layers, the DRZ, and even the Culebra and Magenta aquifers of the Rustler formation. NUTS's transports in the dolomite aquifers are not used in CCA computations, since they are recalculated in greater detail and using more complex assumptions (compound media with retardation processes, for example) by SECOFL2D and SECOTP2D. However, NUTS's transports up the shaft and intrusive boreholes serve as the source terms for the SECOTP2D calculation. In that respect, they interface smoothly and wholly validly, as is described in the section on Culebra flow and transport.

NUTS's calculated lateral transports through the marker beds and anhydrite interbeds are terminal results that must be interfaced only with WIPP's statistical-analysis codes, which is accomplished perfectly within the context of their assumptions.

Units Above the
Salado

1. Model Name

Conceptual model for the geology and hydrology of units above the Salado Fm.

2. Responsible Contacts

P. Davies, A. Lappin, T. Corbet, and R. Beauheim.

3. Model Description and References

The conceptual model used in performance assessment for the units above the Salado Fm. is a simplification of the detailed understanding of the natural system. For each major lithologic unit, the BRAGFLO model specifies layer thickness, important material properties including porosity and permeability, and hydrologic properties such as pressure and initial fluid saturation. For the SECOFL2D and SECOTP2D models of the Culebra Dolomite Member, which is assumed to be the only subsurface pathway for radionuclide transport above the Salado, the conceptual model includes spatial variability in hydraulic conductivity and physical and chemical transport processes. Properties of each unit are chosen to be consistent with available information and with the purpose of the model.

The three anhydrite/mudstone members of the Rustler Fm. (the lower unnamed member, the Tamarisk Member, and the Forty-niner Member) are treated as impermeable layers for BRAGFLO modeling. Field data indicate extremely low permeability in these units, and the assumption that they are impermeable tends to increase the volume of brine that may enter the other units from an intrusion borehole. Parameter values for the other units (the Culebra, the Magenta, the Dewey Lake, and the Santa Rosa and overlying units) are chosen to be consistent with field data. Fluid may flow from an intrusion borehole into each of these units or to the land surface.

Basic stratigraphy and hydrology of the units above the Salado are described in Sections 2.1 and 2.2 of the Compliance Certification Application. Additional supporting information is contained in Appendix GCR and Appendix SUM. Details of the conceptual model for each unit are described in Sections 6.4.6.1 through 6.4.6.7.

4. Model Purpose

The conceptual model for units above the Salado Fm. was developed to provide a reasonable and realistic basis for simulations of fluid flow within the disposal system and detailed simulations of ground-water flow and radionuclide transport in the Culebra. In addition, the conceptual model used for fluid flow is consistent with the conceptual model used in developing the shaft seal design (see Appendix SEAL).

5. Principal Parameters and Relationships among Parameters Defined by the Model

Parameters defined by the conceptual model for each unit are discussed in the relevant subsections of Section 6.4.6.

6. Uncertainty in Conceptual Models and the Relative Significance of Parameters

Climatic recharge was concluded to be a less-important parameter for purposes of 40 CFR 191 (WIPP Performance Assessment Department, 1992b).

7. FEPs Associated with Model Development

See Section 9.

8. History of Model Development and Alternatives Considered and Rejected

The conceptual model used in the WIPP FEIS in 1980 (Lappin et al., 1989, Table 1-1, pp. 1-14 - 1-16) recognized three water-bearing zones within the Rustler Fm., i.e., the Magenta Dolomite, Culebra, and the "Rustler-Salado-interface" (p. 7-87). The Culebra and Magenta, although known to be separate units, were combined for regional-scale transport modeling into a "Rustler aquifer" and assigned a uniform hydraulic conductivity, except in Nash Draw. In the modeling, the Rustler aquifer was assumed to be an isotropic porous medium with a uniform porosity of 0.10 (Table K-2, p. K-18). Regional flow was assumed to be toward the southwest, with discharge at Malaga Bend on the Pecos River. (There was no regulatory framework or boundary defined at that time.) Numerical modeling was not able to consider the possible impact of variations in brine density within the Rustler Fm.; modeling used an equivalent freshwater head. Steady-state flow directions and rates were assumed. Fluid flow in units above the Rustler was not considered because the limited available information suggested that these units were unsaturated. Units below the Castile were assumed to have no effect on performance and were not included in the analysis.

Several developments in the conceptual model took place by 1989 (Lappin et al., 1989; Davies, 1989). Most importantly, interest in fluid flow within the Rustler became strongly focused on the Culebra Dolomite. The Culebra is at least one order of magnitude more permeable than the Magenta Dolomite, except in Nash Draw. Modeling by Barr et al. (1983) showed no significant transport or fluid movement through the Magenta, and none of the hydraulic tests in the Magenta show anything but porous-medium behavior. All other units within the Rustler (unnamed lower member, Tamarisk, Forty-niner) were even less permeable than the Magenta. Both porosity and permeability of the lower Dewey Lake also appear to be significantly lower than the Magenta. In the DSEIS and the December 1992 PA calculations, all fluid flow and transport was assumed to be concentrated in the Culebra; this was thought to be a conservative approach because it did not take credit for flow in other units.

Other important changes in the conceptual model were in place by 1989. The potential for vertical fluid flow within the Rustler was recognized, on the basis of limited data, although for flow and transport calculations, the Culebra was assumed to be perfectly confined. Long-term flow transients within the system, related to climate change, were considered to be likely but were not incorporated into the DSEIS calculations. Modeling boundaries were not arbitrary, but instead coincided with hydrologic features, which revealed the need for three-dimensional flow modeling at the scale of the ground-water basin. Hydrologic properties for the three-dimensional model were inferred from knowledge of geologic processes. Understanding of a water table within the Dewey Lake developed; the position of the water table was assumed move as a function of climatic change. Finally, the possibility of vertical fluid flow in an open borehole between the Rustler and the Bell Canyon was considered, but it was concluded that such fluid flow would be directed downward and was therefore of no physical or regulatory concern.

The December 1992 PA calculations recognized the need for regional-scale modeling. A regional-scale model was used to provide boundary conditions for site-scale flow and transport calculations. A transient flow field was calculated, based on time/climate varying boundary conditions applied at the regional scale. There were no other major changes in modeling approaches; all flow and transport was still forced into the Culebra.

By 1994, flow into lower-permeability units adjacent to shafts and intrusion boreholes was included in modeling. Flow was allowed into the Magenta and Dewey Lake, but with the assumption that actinides would not reach the site boundary through these units. The Project identified the need for modeling to justify the assumption that radionuclides would not migrate significantly within the Dewey Lake (FEP NS-1). Heads and transmissivities within the newly included units were chosen conservatively, i.e., to force most flow into the Culebra Dolomite. A steady-state flow field was used instead of a transient field in the PA model of the Culebra; this was intended to include maximum effects of potential climate variability and was a change in model implementation, not in the conceptual model.

References:

Barr, G.E., W. B. Miller, and D.D. Gonzalez,. 1983. *Interim Report on the Modeling of the Regional Hydraulics of the Rustler Formation.* SAND83-0391. Albuquerque, NM: Sandia National Laboratories.

Davies, P.B. 1989. *Variable-Density Ground-Water Flow and Paleohydrology in the Waste Isolation Pilot Plant (WIPP) Region, Southeastern New Mexico.* Open-File Report 88-490. Albuquerque, NM: U.S. Geological Survey.

Lappin, A.R., R.L. Hunter, D.P. Garber and P.B. Davies, eds. 1989. *Systems Analysis, Long-Term Radionuclide Transport, and Dose Assessments, Waste Isolation Pilot Plant (WIPP),*

Southeastern New Mexico; March 1989. SAND89-0462. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992a. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 2: Technical Basis.* SAND92-0700/2. Albuquerque, NM: Sandia National Laboratories.

WIPP Performance Assessment Department. 1992b. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 4: Uncertainty and Sensitivity Analyses for 40 CFR 191, Subpart B.* SAND92-0700/4. Albuquerque, NM: Sandia National Laboratories.

9. Information Supporting Model Choice and Confirmation

NS-1, Transport within the Dewey Lake. After analysis it was concluded that radionuclide transport within the Dewey Lake could be neglected.

NS-2/3, Passive interconnections within and outside the controlled area. It was concluded that vertical fluid flow as a result of drilling (not including pumping or injection of fluids) could be neglected on the basis of negligible consequence.

NS-4b/5b, Pumping from the Dewey Lake inside and outside the controlled area.

NS-7, Leakage from wells (brine pockets, injection wells, fluids released during drilling). It was concluded that this phenomenon could be neglected on the basis of low consequence.

NS-8, Natural Climate Change. It was concluded that PA calculations should continue to consider the potential impacts of climate change.

NS-9, Justification of the SECO 2D Approximation for Culebra Flow and Transport. It was concluded that PA was justified in using a completely confined two-dimensional flow and transport model for the Culebra.

NS-10, FEPs Leading to Localized Changes in Recharge. It was concluded that such localized recharges could be neglected on the basis of low consequence.

NS-21, Connections to Units Beneath the Repository. It was concluded that this could be neglected on the basis of having no consequence.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See summary notes on the conceptual model for fluid flow in units above the Salado Formation (CCA Sections. 6.4.6.1, 6.4.6.3, 6.4.6.4, 6.4.6.5, 6.4.6.6, and 6.4.6.7).

Culebra

1. Model Name

Conceptual model for ground-water flow in the Culebra Member of the Rustler Formation.

2. Responsible Contacts

J. Ramsey, P. Davies, A. Lappin, L. Meigs, and R. Beauheim.

3. Model Description and References

The conceptual model used in performance assessment for ground-water flow in the Culebra treats the Culebra as a confined two-dimensional aquifer with constant thickness and spatially varying transmissivity. Flow is modeled as single-phase (liquid) Darcy flow in a porous medium.

Basic stratigraphy and hydrology of the units above the Salado are described in Sections 2.1 and 2.2 of the Compliance Certification Application. Additional supporting information is contained in Appendix GCR and Appendix SUM.

The conceptual model for flow in the Culebra is discussed in Section 6.4.6.2. Details of the calibration of the transmissivity field, based on available field data, are given in Appendix TFIELD. Initial and boundary conditions used in the model are given in Section 6.4.10.2.

4. Model Purpose

The conceptual model for ground-water flow in the Culebra provides a reasonable and realistic basis for simulating radionuclide transport in the Culebra and allows evaluation of the extent to which uncertainty about ground-water flow in the Culebra may contribute to uncertainty in the estimate of cumulative radionuclide releases from the disposal system.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The principal parameter used in the performance assessment to characterize flow in the Culebra is an index parameter (the transmissivity index) used to select a single transmissivity field for each Latin hypercube sample element from a set of calibrated fields, each of which is consistent with available data.

Generation of the transmissivity fields is discussed in Appendix TFIELD.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Sensitivity analyses performed as part of the 1992 preliminary PA identified the relative importance of sampled parameters with respect to human-intrusion scenarios and undisturbed performance. For human intrusion, parameters were ranked as follows (WIPP Performance Assessment Department, 1992, pg. 9-8):

- two parameters were considered critically important; neither was from the Culebra;
- five parameters were considered very important, including Culebra fracture spacing #4;
- two parameters were considered important, including Culebra transmissivity field #1 and matrix porosity #2;
- twenty-four parameters were considered less important, including Culebra fracture porosity.

In the 1992 preliminary PA, a comparison of single-porosity (fracture-only) versus dual-porosity behavior indicated a one- to two-order of magnitude increase in integrated release for fracture-transport only.

Reference:

WIPP Performance Assessment Department. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 4: Uncertainty and Sensitivity Analyses for 40 CFR 191, Subpart B*. SAND92-0700/4. Albuquerque, NM: Sandia National Laboratories.

7. FEPs Associated with Model Development

See Section 9.

8. History of Model Development and Alternatives Considered and Rejected

Since the Final Environmental Impact Statement (FEIS) in 1980, the conceptual model used to describe flow and transport within the Culebra has changed significantly. In the FEIS, the Culebra and Magenta Dolomite Members were combined and modeled as one layer referred to as the "Rustler aquifers." In the modeling, the "Rustler aquifers" were assumed to be an isotropic porous medium with a uniform porosity of 0.10 (Lappin et al., 1989, Table K-2, p. K-18). A uniform transmissivity field was assumed across the model domain except in Nash Draw. Regional flow was assumed to be toward the southwest discharging at Malaga Bend on the Pecos River. (There was no regulatory framework or boundary defined at this time.) Numerical modeling was not able to consider the possible effect of variations in brine density within the Rustler, so modeling used an equivalent freshwater head; the model was unable to consider possible effects of brine density on ground-water flow. Steady-state flow directions and rates were assumed. As for physical-transport characteristics, the Culebra was incorporated into the "Rustler aquifers" and assumed to be an isotropic, homogeneous porous medium.

In 1987, a new model (Haug et al., 1987) used a more-developed conceptual model of the Culebra flow domain. This study calibrated a flow model to the H-3 pumping test and the effects from the excavation of the shafts. Data from numerous new boreholes installed and tested since the 1980 study were included in this model. The boundaries of the model were not much larger than the extent of the WIPP site. Brine densities were also used as a calibration target. The brine densities were assigned at the boundaries and subsequently modified to match the observed fluid densities. Vertical recharge was included in an attempt to calibrate the brine densities. The transmissivity field was estimated by kriging and modified by the addition of pilot points, which

were located by trial and error. In this model, single- and dual-porosity effects on the flow field were investigated. At the regional scale, the use of a dual-porosity vs. single-porosity conceptual model had little effect on the flow field.

A modeling study conducted to support the DSEIS (Lavenue et al., 1989) only slightly modified the conceptual model used by Haug et al. (1987). The difference in the conceptual model was the assumption that brine density was variable but fixed over the time scale of the model (i.e., ten years). It was assumed that the brine concentrations could be considered at a quasi-steady state over this period of time. The boundaries of the 1989 study were much larger than those of the 1987 study, extending ~30 km north and south and 20 km in east and west. The model grid was centered on the WIPP site. The boundaries were selected to maximize the use of regional freshwater heads and to minimize the boundary effects during transient simulation of the H-3, WIPP-13, and H-11 pumping tests. Vertical recharge was not included. Fixed heads were assigned around all four boundaries based upon the regional head values. Transmissivities were estimated by kriging and ranged over seven orders of magnitude in this study. Pilot points were added to modify the transmissivity field during steady-state and transient calibration. Pilot-point locations were selected using an adjoint sensitivity analysis technique.

By the time of the draft Supplemental Environmental Impact Statement (DSEIS) (Lappin et al., 1989), the conceptual model of the Culebra Dolomite had changed. The Culebra transmissivity field was calibrated on the basis of 41 test locations. Transmissivity was recognized to vary by approximately three orders of magnitude within the WIPP site. Modern flow in Culebra is predominately north to south on the site, but it is dominated by a high-transmissivity zone in the southeastern portion of the site. Flow was calculated on the basis of a fully confined Culebra and boundary conditions applied at the site scale. Local flow and transport behavior were affected by fracturing (dual-porosity hydraulic response) where the transmissivity is greater than $\sim 10^{-6}$ m^2/s. For physical transport, a double-porosity (matrix-diffusion) transport conceptual model for off-site transport from waste panels was assumed. Transport parameters were based on best estimates from non-sorbing tracer tests at three locations. It was assumed that the effective thickness was equal to the total thickness. Contaminant-transport calculations for the DSEIS were one-dimensional.

The initial conditions for the Culebra flow field have been taken from the hydrographs of the WIPP boreholes. Prior to excavation of the first shaft (i.e., the Control and Salt Handling Shaft), the hydrographs depicted a quasi-steady state flow field over the ten to twenty years preceding the shaft excavations. Head values were selected for each borehole with a hydrograph that preceded shaft excavation or that was located far from the shaft effects on the flow field. These data provided an estimate of the undisturbed head field and were subsequently used as initial conditions for the Culebra model's transient simulation.

In modeling the hydrologic characteristics of the Culebra, the December 1992 PA calculations generated multiple transmissivity fields conditioned on hydraulic test data and then sampled those fields. This procedure addressed uncertainties in the location-specific values of the Culebra transmissivity. The geologic conceptual model was further revised to indicate that the degree of fracture flow was related to the degree of gypsum cement removal. Contaminant-

transport calculations were two-dimensional. The effective thickness of the Culebra was taken to be equal to the total thickness. A range of physical-transport parameters was used, as opposed to best estimates, to address the variability of physical-transport properties within the Culebra. The maximum fracture spacing was assumed to be equal to the total thickness of the Culebra (~8 m). The fracture spacing assigned in the PA modeling greatly simplified reality. In reality, the Culebra Dolomite probably does not contain through-going parallel fractures. Representing fracturing in terms of fracture spacing is a mechanism to ensure that the proper surface-to-volume ratios are used in estimating the role of matrix diffusion. Calculations considered the possibility of both single-porosity (fracture-flow-only) and dual-porosity (matrix diffusion) behavior.

Multiple transmissivity fields were generated and subsequently calibrated to the same steady-state and transient events used in the 1989 model. The main differences between the 1989 and 1992 models were the model boundary locations, boundary conditions, and the geostatistical approach used to develop and modify the transmissivity field. The 1992 model boundaries were rotated 38 degrees east to align with the axis of Nash Draw. This permitted the specification of a no-flow boundary along a portion of the western boundary coinciding with the Nash Draw axis. In addition, the northeastern corner of the model was a no-flow boundary because of the low transmissivities in the area and the lack of any nearby regional heads to provide boundary head estimates. Transmissivities were simulated by conditional simulation. Pilot points were automatically located and assigned transmissivity values using an optimization routine during steady-state and transient-state calibration.

By 1994, the conceptual model of the Culebra's hydrologic characteristics was unchanged from that of December 1992. For the physical-transport characteristics, dual-porosity transport was assumed, but the base case had large fracture spacing, effectively the same as the Culebra thickness. A single block size was assumed in each realization. Calculations still assumed an effective thickness equal to the total thickness.

Since 1994, the conceptual model of the Culebra's regional hydrologic characteristics has not changed, although additional large-scale information from pumping at H-19 has been incorporated into the calibration. Existing borehole-transmissivity interpretations have been refined. The conceptual model of the physical-transport characteristics has changed on the basis of analysis of new data from H-19 and H-11 and reanalysis of previous tests of H-3, H-11, H-6. The Culebra is now conceived of as a fractured porous medium with inherent local variability in the degree and scale of fracturing. This is transmitted to the PA team in terms of a "matrix block length" that gives the correct surface-to-volume ratio for diffusion. Culebra porosity consists of intergranular porosity, microfractures, vugs, and macroscopic fractures. This variability leads to both lateral and vertical variations in permeability. Advection is believed to occur largely through fractures; however, in some areas it may also occur through vugs connected by small fractures. Inputs to PA, rather than being conceived of in terms of fracture and matrix porosities, are conceived of as "advective" and "diffusive" porosities. Matrix diffusion is still believed to be effective and significant. The effective transport thickness is thought to be less than the total stratigraphic thickness. The limited available data suggest that the permeability of the upper portion of the Culebra is relatively low. The Project has concluded that the Culebra is adequately

represented by a dual-porosity model on the scale of PA calculations; it is not necessary to use a discrete-fracture model on this scale.

Reference:

WIPP Performance Assessment Department. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 4: Uncertainty and Sensitivity Analyses for 40 CFR 191, Subpart B*. SAND92-0700/4. Albuquerque, NM: Sandia National Laboratories.

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LaVenue, A.M., A. Haug, and V.A. Kelley. 1988. *Numerical Simulation of Ground-Water Flow in the Culebra Dolomite at the Waste Isolation Pilot Plant (WIPP) Site. Second Interim Report*. SAND88-7002. Albuquerque, NM: Sandia National Laboratories.

9. Information Supporting Model Choice and Confirmation

NS-4a/5, Pumping from Culebra inside and outside the controlled area. It was decided that both events could be neglected based on regulatory arguments.

NS-9, Justification of SECO2D Approximation for Culebra Transport Calculations. It was concluded that two-dimensional calculations are adequate.

NS-16, Effects of Vertical Heterogeneity on Groundwater Flow Within the Culebra. It was concluded that H-19 testing did support inclusion of vertical heterogeneity within the Culebra. This was done by assigning a decreased effective thickness.

NS-17, 18, 19, 20, Variations in Brine Density Within the Culebra. All of these considerations were screened out on the basis of low consequence.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See Summary Notes on Conceptual Model for Fluid Flow and Physical Transport of Contaminants in the Culebra Dolomite (CCA Section 6.4.6.2).

Dissolved Actinide
Transport in the
Culebra

1. Model Name

Dissolved Actinide Transport in the Culebra.

2. Responsible Contacts

Fluid flow and physical retardation: L. Meigs
Chemical retardation: L. Brush

3. Model Description and References

The properties of the Culebra Dolomite Member of the Rustler Fm. have been characterized by direct observation in outcrop, boreholes, and shafts (Holt and Powers, 1984, 1986, 1988, 1990), field hydraulic testing and analysis (Beauheim, 1987), field tracer testing and analysis (memoranda in CCA; Mercer and Orr, 1979), and laboratory testing and analysis (Papenguth and Behl, 1996a, 1996b).   The conceptual model for dissolved actinide transport in the Culebra is based on these observations, tests, and analyses. Because the conceptual model is based on such extensive analysis and includes for clarity specific terminology developed in the analysis of test results, it is recommended that the reader be familiar with the discussion of Culebra characterization that appears in Sections 2.1, 2.2, and 6.4.6 of the CCA.

The conceptual model for actinide transport in the Culebra has three principal components: advective transport, physical retardation, and chemical retardation. Two types of porosity are present—porosity in which advective transport occurs, and porosity that is relatively inactive in advective transport. This type of behavior is typically referred to as double porosity. Because testing and analysis of the Culebra suggests that its upper portion does not play a significant role in transport, transport is modeled only for the lower portion of the Culebra.

Advective transport refers to the transport of actinides in those pores of the Culebra where the principal fluid flow occurs. This primarily occurs in fractures, but may also occur in vuggy regions or other portions of the porosity of the Culebra that contain large pore-throat apertures. This mechanism includes the effects of diffusion and dispersion in advective porosity as well as the movement of actinides with the bulk fluid flow. Advective transport is thought to be controlled by hydraulic gradient, hydraulic conductivity, thickness, and advective porosity.

Physical retardation refers to the process of diffusion from advective porosity into diffusive porosity, i.e., those portions of the porosity of the Culebra that are relatively inactive in advective transport. Once in the diffusive porosity, the actinides are no longer carried along by the most rapidly moving liquids, and their rate of movement decreases. The properties that control the diffusion of actinides into the diffusive porosity are the surface area between advective porosity and the diffusive porosity, the tortuosity of the diffusive porosity, and diffusion coefficients.

Chemical retardation refers to the sorption of actinides on minerals present in the Culebra. For the most part, the sorption is thought to occur on dolomite grains, but some may also occur on clay or other minerals. Chemical retardation occurs only in the diffusive porosity. The

governing properties for sorption are thought to be the concentration of actinides in solution, the density of minerals on which sorption can occur, and a parametric expression of the degree to which dissolved actinides tend to sorb or remain in solution (in the mathematical model, a K_d for a linear isotherm is used).

Advective porosity is thought to be a small percentage of the total volume of the Culebra involved in transport. This porosity is interconnected and contains high-permeability features such as fractures or vuggy pore structures. In this advective porosity, little actual rock material is considered to exist (in other words, it is the fracture apertures and pore volumes without surrounding rock). In contrast, diffusive porosity makes up the major portion of the Culebra volume. It comprises low permeability features and most of the rock material. An important assumption is that there is a characteristic dimension or length, the units of which are specific to the mathematical model used, that expresses the manner in which the advective porosity intertwines through the diffusive porosity. In the mathematical model used for WIPP, this is called the matrix block length.

In summary, the conceptual model for dissolved actinide transport in the Culebra includes two types of porosity; advective porosity associated with high-permeability features of the Culebra, and diffusive porosity associated with low-permeability features. Advection, diffusion, and dispersion of dissolved actinides occurs within the advective porosity. Diffusion (physical retardation) and sorption (chemical retardation) occurs within the diffusive porosity. Advective porosity makes up a small portion of the overall volume of the Culebra, and an important conceptual model is that of the intertwining or interface between the two porosities, which in part controls how much actinide can enter the diffusive porosity. Because the upper portion of the Culebra has been observed to be unimportant in solute transport in tests, it is not included in the conceptual model.

References:

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Papenguth, H.W., and Y.K. Behl. 1996a. *Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant*, SNL Test Plan TP 96-01.

Papenguth, H.W., and Y.K. Behl. 1996b. *Test Plan for Evaluation of Dissolved Actinide Retardation at the WIPP*. Albuquerque, NM: Sandia National Laboratories.

4. Model Purpose

The purpose of this model is to represent the effects of advective transport, physical retardation, and chemical retardation on the movement of actinides in the Culebra.

5. Principal Parameters and Relationship among Parameters Defined by Model

Several parameters are referred to or implied in the conceptual model. For transport in advective porosity, the principal parameter is the porosity of the network, but because of links to the Culebra fluid flow model, the hydraulic gradient and hydraulic conductivity largely control the specific discharge calculated by SECOFL2D. Within diffusive porosity, the porosity, tortuosity, and diffusion coefficients for various actinides are important because of their effect on the rate of diffusion. A parameter called matrix block length, a measure of the surface area between the advective and diffusive porosities, is also important. The density of sorbing minerals and their sorption properties, expressed by K_d (the distribution coefficient), are important in chemical retardation.

It is commonly assumed that there should be a relationship between the conductivity of advective porosity and its porosity and distribution, that is, that the fracture permeability, porosity, and aperture or spacing should be correlated. Data collected and analyzed at the WIPP do not support this assumption. There is no meaningful trend among these parameters for the data that have been collected. Therefore, values of these parameters are not correlated in the performance assessment.

Transport of actinides in the Culebra is coupled to several other conceptual models. An important coupling is to models for features that can introduce actinides to the Culebra, e.g., the exploratory borehole, shafts and shaft seals, and dissolved actinide source term. The most important coupling is to the model for flow in the Culebra. Because transport in the Culebra is one of the last processes to occur along this pathway prior to potential release, it does not feed back to other conceptual models in any significant manner. In a manner of speaking, this conceptual model falls at the downstream end of the overall disposal system model, and thus has little or no impact on models that come before it.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Several factors affect the sorption of Pu, Am, U, Th, and Np, the elements for which PA personnel require K_ds for Culebra transport calculations (Ramsey, 1996):
- the properties of the sorbents (solids) that will sorb actinides from solution;
- the composition of solutions that currently exist in the Culebra Dolomite or could enter the Culebra after human intrusion into WIPP disposal rooms;
- the oxidation state of the sorbate (actinide elements) in the Culebra;
- dissolved actinide concentration;
- equilibration time; and
- direction of reaction (sorption versus desorption).

The Dissolved Actinide Chemical Retardation Research Program (RRP) has carried out three laboratory studies to investigate these factors: an empirical sorption study by I. Triay and her colleagues at Los Alamos National Laboratory (LANL) (in progress); a mechanistic sorption study by P. V. Brady and his colleagues at Sandia National Laboratories (SNL) and LANL (in progress); and a transport study with intact Culebra cores by D. A. Lucero and his colleagues at SNL (in progress).

The two most important sorbents in the Culebra are dolomite, a carbonate mineral that constitutes most of the Culebra, and corrensite, an ordered mixture of chlorite and saponite associated with fracture surfaces and dispersed in the matrix (intact rock between the fractures) of the Culebra. Dolomite is important because it is by far the most abundant mineral in the Culebra. Corrensite is important because, although a minor constituent, it sorbs actinide elements much more strongly than dolomite. The work of Sewards (1991), Sewards et al. (1991, 1992), and recent, unpublished studies of Culebra mineralogy indicate that corrensite is associated with fracture surfaces and dispersed in the matrix at concentrations high enough to increase the retardation of Pu, Am, U, Th, and Np relative to that observed in laboratory studies with nearly pure dolomite. However, the Project does not plan to include K_ds for clay minerals in the ranges and probability distributions for the matrix K_ds for use in the PA calculations to support the WIPP CCA because laboratory data for clay-rich rock under expected Culebra conditions are insufficient at this time. Furthermore, the Project does not plan to take any credit for sorption by clay minerals associated with fracture surfaces. Omitting K_ds for clays appears to be conservative.

The composition of solutions that currently exist in the Culebra or that could enter the Culebra after human intrusion could also affect actinide sorption. The RRP has used four synthetic fluids, Brine A, ERDA-6, AISinR, and H-17, in its laboratory studies. Brine A (Molecke, 1983) is similar to intergranular Salado-Formation brines at or near the stratigraphic horizon of WIPP disposal rooms. These brines could flow from the repository into the Culebra in the event of human intrusion. ERDA-6 (Popielak et al., 1983) simulates brines that occur in isolated but occasionally large reservoirs in the Castile Formation. These brines could also 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. H-17 simulates Culebra brine from the H-17 Hydropad. The RRP has also studied the effects of the partial pressure of CO_2

(and hence dissolved CO_2 concentration and, to some extent, pH) on sorption. Triay has 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. These four atmospheres have had CO_2 partial pressures of $10^{-3.5}$, $10^{-2.73}$, $10^{-1.98}$, and $10^{-1.50}$ atm, respectively, the range of P_{CO2} calculated for Culebra ground waters by Siegel et al. (1991). Brady has also studied the effects of CO_2 partial pressure (in progress). Furthermore, Brady studied the effects of ionic strength, pH, and the concentrations of potentially significant cations and anions.

These studies have quantified the effects of solution composition on sorption. However, the extent to which deep (Castile and Salado) and Culebra brines mix along the flow path from the point of injection of deep brines into the Culebra to the boundary of the Land Withdrawal Area has not yet been predicted. Therefore, weighting factors to combine the ranges and probability distributions of K_ds established for deep and Culebra brines and to obtain an overall range for a given element or elemental oxidation state have not been specified. Consequently, the Project is taking the following, conservative approach: (1) establish *separate* ranges and probability distributions of actinide K_ds for the deep and the Culebra brines; (2) instruct PA to use the ranges and probability distributions of actinide K_ds that result in less retardation for a given element or elemental oxidation state.

The oxidation state of the actinide elements significantly affects their chemical behavior, including sorption. Papenguth and Behl (1996) state that, in general, the relative tendency of the actinide elements to sorb is An(IV) > An(III) ~ An(VI) > An(V), where "An" is the abbreviation for actinide elements such as Pu, Am, U, Th, and Np, and the Roman numerals III, IV, V, and VI indicate the +3, +4, +5, and +6 oxidation states. Therefore, the RRP has investigated the effects of oxidation state on actinide sorption and predicted the oxidation-state distributions of Pu, U, and Np in the Culebra. So far, results from the empirical sorption study, the mechanistic sorption study, and the transport study imply that the relative sorption tendency under expected Culebra conditions is An(IV) > An(V) > An(VI). (Acceptable sorption data for Am(+3) are not yet available.) The following oxidation states in the Culebra are expected For Pu, U, and Np,: Pu(+3) and Pu(+4); U(+4) and U(+6); and Np(+4) and Np(+5). For Am and Th, only one oxidation state, Am(+3) or Th(+4), is possible.

Triay has studied the effects of dissolved actinide concentration on sorption (in progress). These experiments have yielded sorption isotherms, plots of the quantity of radionuclide sorbed by the solid phase or phases versus the final dissolved radionuclide concentration, or plots of K_ds versus the final dissolved radionuclide concentration. These plots have in turn provided information on the nature of the reaction(s) responsible for removing radionuclides from solution. Finally, Triay studied the effects of equilibration time and direction of reaction (sorption or desorption) on sorption. She has conducted 3-day, 1-week, 3-week, 6-week, and 8-week sorption and desorption experiments.

Currently the greatest source of uncertainty in the predictions of actinide sorption is probably the extent to which deep (Castile and Salado) and Culebra brines mix along the flow

path. Because of this uncertainty, the Project is following the conservative approach described above.

7. FEPs Associated with Model Development

RNT-11, hydrogeochemical changes caused by injection of deep (Castile or Salado) brines into the Culebra

RNT-13, effects of nonlinear, irreversible on sorption in the Culebra

RNT-14, effects of solution composition on sorption in the Culebra

RNT-18, effects of dissolved-actinide speciation on sorption in the Culebra

RNT-19, solubility effects in the Culebra

8. History of Model Development and Alternatives Considered and Rejected

The WIPP Project carried out several laboratory studies of sorption in the late 1970s and early 1980s (Serne et al., 1977; Paine and Dosch, 1992; Dosch and Lynch, 1978; Dosch, 1979, 1980, 1981; Lynch and Dosch, 1980; Lynch et al., 1981; Tien et al., 1983). These empirical studies used a variety of sorbents and solutions—including dolomitic, anhydritic, and clay-rich rocks and repository and Culebra brines—and in some cases included the effects of dissolved organics on sorption. The DOE (1980) used some of these results for the 1980 WIPP Environmental Impact Statement (EIS). According to Lappin et al. (1989), the sorption model used by the DOE (1980) included a porous-medium approximation of the Culebra. Lappin et al. (1989) and the DOE Office of Environmental Restoration and Waste Managment (1990) also used these results for the 1990 Supplemental EIS. For Pu, Am, U, Th, Np, and Cm, Lappin et al. (1989) and the DOE Office of Environmental Restoration and Waste Managment (1990) included sorption by the matrix only, linear sorption isotherms, and instantaneous, reversible equilibrium in their model. For Ra and Pb, however, they assumed linear, instantaneous, reversible sorption by clay minerals in the matrix because there were no data available for sorption of these elements by dolomite.

During the middle 1980s, the DOE and the State of New Mexico formally recognized deficiencies in the early sorption studies cited above. In 1988, they modified the Consultation and Cooperation (C&C) Agreement to require additional sorption studies for the WIPP Compliance Certification Application. Papenguth and Behl (1996) planned the current program (see below) in part to satisfy that agreement. The C&C Agreement stipulates that DOE recognizes that radionuclide retardation within the Culebra remains to be proven experimentally and remains committed to demonstrate experimentally the actual range of K_ds to be expected for transport within the Culebra. It is unlikely that transport will involve a single set of K_d values, and performance assessment likely must consider a range of values for each element. DOE will select, after consultation with the State, a range of values to be conservative, but reasonable, based on the lowest reasonable values experimentally obtained. In the absence of experimentally justifiable values, K_d will equal zero, i.e., no credit for retardation will be taken in the performance assessment calculations.

Soon after the C&C Agreement was reached, the WIPP Project started a mechanistic sorption study, primarily at Stanford University (Lappin et al., 1989; Siegel et al., 1990; Park et al., 1992, 1995). The objective of this study is to develop a surface-complexation model for the sorption of UO_2^{2+} by corrensite, the dominant clay mineral in the Culebra. It is infeasible, however, to use this model in the PA calculations for three reasons:

- laboratory data for clay-rich rock under expected Culebra conditions are insufficient at this time to include K_ds for clay minerals in the PA calculations to support the WIPP CCA;
- the Stanford results pertain only to sorption of U(+6) and its oxidation-state analogs Pu(+6) and Np(+6), none of which will significantly affect the long-term performance of the WIPP; and
- even if sorption of U(+6), Pu(+6), or Np(+6) did affect the long-term performance of the WIPP significantly, it would not be possible to incorporate a surface-complexation model in the Culebra flow and transport code SECO.

At about the same time that the Stanford mechanistic sorption study began, the WIPP Project convened an expert panel consisting of SNL staff to estimate ranges and probability distributions of K_ds for use in probabilistic PA calculations for the WIPP. This panel estimated ranges and distributions of actinide K_ds for the Culebra as a whole and for the clay-rich fracture surfaces (Trauth et al., 1992). PA personnel used these values for their 1991 and 1992 calculations.

In March 1995, the RRP began to obtain K_ds for use in the PA calculations to support the WIPP CCA. This program, described by Papenguth and Behl (1996), has included an empirical sorption study by Triay at LANL, a mechanistic sorption study by Brady at SNL and LANL, and a transport study by Lucero at SNL (see Relative Significance of Parameters above). Papenguth and Behl (1996) planned to use the results of these studies to evaluate alternative conceptual models of Pu, Am, U, Th, and Np retardation by the Culebra, such as the relative extent to which the dolomitic matrix and the clay-rich fracture surfaces sorb these elements, predictions of brine mixing and the effects of solution composition on sorption, predictions and effects of the oxidation-state distributions of Pu, U, and Np, and the effects of dissolved actinide concentration on sorption. In particular, Papenguth and Behl (1996) hoped to use the results of experiments carried out with various dissolved Pu, Am, U, Th, and Np concentrations to specify whether PA should use linear, Langmuir, or Freundlich sorption isotherms for these elements in its Culebra transport calculations.

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9. Information Supporting Model Choice and Confirmation

The RRP has amassed a large database on the effects of several factors on the sorption of Pu, Am, U, Th, and Np by nearly pure dolomite in the matrix of the Culebra. Although corrensite is thought to be present on fracture surfaces and in the matrix at concentrations high enough to increase the retardation of Pu, Am, U, Th, and Np, laboratory data for clay-rich rock are insufficient at this time to include K_ds for clay minerals in the ranges and probability distributions for K_ds for use in the PA calculations to support the WIPP CCA.

Similarly, although the RRP has quantified the effects of solution composition on sorption, the extent to which deep (Castile and Salado) and Culebra brines mix after human intrusion is unknown. The Project is taking the conservative approach of establishing separate ranges and probability distributions of actinide K_ds for the deep and the Culebra brines and instructing PA to use the ranges and probability distributions that result in less retardation, rather than specify weighting factors to combine the ranges and probability distributions established for these brines.

Finally, Triay quantified the effects of dissolved Pu, U, Th, and Np concentration on the K_ds for these elements in six-week sorption experiments. However, it has not been possible to use the results to specify the nature of the sorption isotherms for these elements for the PA calculations, because the Culebra transport code SECOTP2D can use linear sorption isotherms but not Langmuir and Freundlich isotherms as anticipated by Papenguth and Behl (1996).

Reference:

Papenguth, H.W., and Y.K. Behl. 1996. *Test Plan for Evaluation of Dissolved Actinide Retardation at the Waste Isolation Pilot Plant.* TP 96-02. Albuquerque, NM: Sandia National Laboratories.

10. Validity and Completeness

The RRP has attempted to ensure the validity and completeness of its results by using complementary approaches to quantify actinide sorption under expected Culebra conditions. For example, results from Triay's empirical sorption study (in progress) formed the basis for establishing ranges and probability distributions of matrix K_ds for Pu, Am, U, Th, and Np for use in the PA calculations to support the CCA, because the simplicity of these experiments allowed Triay to quantify the effects of a variety of factors on sorption. However, results from Brady's

mechanistic sorption study, which minimized the effects of factors such as dolomite dissolution, actinide precipitation, and other reactions unrelated to sorption, were also used to help interpret the results of the empirical sorption study and to extend the empirical results to the basic conditions expected to result from use of an MgO backfill in WIPP disposal rooms.

Furthermore, the results of the empirical study agree well with those of Lucero's transport study (in progress) with intact Culebra cores. This implies that the K_ds measured in empirical batch experiments can be used to predict the sorption of Pu, Am, U, Th, and Np from synthetic Castile or Culebra brines flowing at rates at or close to the upper limit of the range of *in situ* fluid velocities through intact, well preserved Culebra cores obtained from horizontal boreholes aligned in the current direction of ground-water flow in the Culebra.

Climate Changes

1. Model Name

Conceptual model for evaluating effects of future climate change on the long-term performance of the WIPP.

2. Responsible Contacts

T. Corbet and P. Swift.

3. Model Description and References

Paleoclimatic data from the literature form the basis for reconstructing the climatic variability in southeastern New Mexico since late Pleistocene time, spanning the transition from full glacial conditions in North America (ice sheets as far south as the Northern Great Plains) to the present interglacial period. The wettest and coolest climate at the WIPP corresponded to periods of continental glaciation. During Holocene time (the past 10,000 years), the climate has been predominantly dry, like that of the present, with several wetter episodes.

Future climate at the WIPP may differ in the next 10,000 years from that of the present, but it should be bounded by the extremes of the late Pleistocene glaciation. For the purposes of performance assessment, the DOE assumes that uncertainty about future climate is adequately captured by considering two possible patterns: one in which the Holocene pattern of predominantly dry conditions alternating with wetter conditions continues; and one in which the climate becomes continuously wetter.

Effects of climatic change on the WIPP are limited in the performance assessment model to effects on ground-water flow in the Culebra Dolomite. Flow (i.e., specific discharge in the SECOFL2D model) is increased from its present calibrated value by a sampled factor that ranges from 1.0 to 2.25 to simulate effects of wetter climates. Possible decreases in flow during drier climates are not considered. Justification for limiting the effects of climate change to flow in the Culebra is based on regional three-dimensional modeling that estimates the extent to which changes in recharge will alter the altitude of the water table and in turn affect flow in the Culebra and other units. Maximum recharge rates considered in the analysis result in a simulated water-table altitude at or near the ground surface throughout the region. Other effects of climatic change, including changes in temperature, wind, evapotranspiration, and vegetation, are not modeled explicitly but are qualitatively included in this analysis through the consideration of the effects of varying recharge.

References:

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See also:

Section 6.4.9, Section 2.5, Appendix CLI, Appendix SCR Section SCR.1.6, Appendix PAR, and references listed under items 6 through 10.

4. Model Purpose

The purpose of this model is to allow quantitative consideration of the extent to which uncertainty about future climate may contribute to uncertainty in estimates of cumulative radionuclide releases from the disposal system. Consideration is limited to conditions that could result from reasonably possible natural climatic changes. The model is not intended to provide a quantitative prediction of future climate, nor is it intended to address uncertainty in system properties other than estimated cumulative radionuclide releases that may be affected by climate change.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The climate change model is implemented through the use of a single parameter, the Climate Index. This parameter is a dimensionless factor by which the specific discharge in each grid block of the SECOFL2D domain is multiplied. It is a sampled parameter in the performance assessment, with a bimodal distribution ranging from 1.00 to 1.25 and from 1.50 to 2.25. See Section 9 for a reference for the justification for this distribution.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The climate change model used for performance assessment is predicated on the assumption that climate will change during the next 10,000 years. The extent of this change is uncertain, but it should be bounded by the changes that occurred in the past during the peaks of Pleistocene glaciation. Other conceptual models for climate change are not consistent with present scientific understanding of the Earth's climate or with the EPA's guidance to consider "natural processes" of climatic change (EPA, 1996, p. 5227). For example, climate could be assumed to remain constant for 10,000 years, but this would be inconsistent with scientific understanding of climate. Alternatively, climate could be assumed to change to conditions unlike any known from the Pleistocene; however, no natural processes are known that could result in such change within 10,000 years.

As discussed in the memorandum attached to Section 9 below, the implementation of climate change in the performance assessment incorporates uncertainty about future climates within the range known from the Pleistocene. Alternative approaches to treating climate change in the performance assessment (i.e., varying boundary conditions rather than specific discharge)

are discussed in Section 8. Past analyses performed using a different approach as part of the 1991 and 1992 preliminary performance assessments suggest that disposal system performance is not sensitive to climate change (Swift et al., 1994, p. 12).

Reference:

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7. FEPs Associated with Model Development

NS-8a and NS-8b, Climate Change
NS-9, Two-Dimensional Assumption for Culebra Calculations

8. History of Model Development and Alternatives Considered and Rejected

Past changes in climate at the WIPP have been recognized since the earliest site characterization work. As described in Appendix GCR (page 3-102), Brokaw et al. (1972) and Bachman (1974) interpreted the sedimentary record of the Gatuña Formation, the Mescalero caliche, and the overlying surficial sediments (see Sections 2.13.8., 2.1.3.9, and 2.1.3.10) as indicating alternating wetter and drier climates during the Pleistocene. Bachman continued extensive geologic work in the WIPP region throughout site characterization and further documented the sedimentary evidence for Pleistocene climatic change (Bachman, 1976, 1980, 1981, 1984, 1985, 1987). One borehole, WIPP-15, was drilled in 1978 in San Simon Sink southeast of the WIPP to examine the causes of subsidence in the sink and to obtain paleoclimatic data (Sandia National Laboratories and University of New Mexico, 1981). Core from the borehole indicates about 547 feet of total subsidence in the Quaternary. Aquatic fauna and flora from the upper 98 feet of core indicate a wet climate followed by an arid period before the present.

In addition to site-specific geologic evidence, past climatic changes have been inferred by other workers throughout the southwest based on various data. Bachman (1989) prepared an annotated bibliography of relevant information published as of 1984. Swift (1993, reproduced in the Compliance Certification Application as Appendix CLI) prepared a synthesis of Pleistocene climate at the WIPP based on detailed examination of available literature. Swift's analysis forms the basis for the present understanding of climatic change.

Early interest in the possible effects of climatic change on disposal system performance focused on the possibility that wetter climates might increase rates of salt dissolution. As discussed in Section 2.1.6.2 and Appendix SCR Section SCR.1.1.5.1, average dissolution rates

over the past several hundred thousand years include both wet and dry climates and are too low to affect disposal system performance during the next 200,000 years. Questions have also been raised about whether dissolution or precipitation of fracture fillings in the Culebra could occur during climatic changes and alter the rate of radionuclide transport in ground water. As discussed in Appendix SCR.1.1.5.2, isotopic data from Siegel et al. (1991, p. 5-53 through 5-57), Chapman (1986), and Lambert (1987) indicate that mineralogical changes from interactions with ground water have been minimal during late Pleistocene time in the units above the Salado. Future mineralogical changes that might occur during climate changes are therefore also expected to be minimal.

Based on their interpretation of uranium isotope activity ratios and other isotopic data from WIPP-area ground water, Lambert and Carter (1987) and Lambert (1991) proposed that climatic change in the past could have had a significant effect on ground-water flow direction. In their interpretation, wetter conditions during the late Pleistocene recharged the Rustler Formation in the vicinity of Nash Draw, with flow occurring to the southeast. Drier conditions of the Holocene (including the present) resulted in no recharge and a gradual shift in flow directions to those observed at present.

Current understanding of regional ground-water flow is consistent with Lambert and Carter's general observation that flow directions may change with changing climate, but the specifics of their proposal are not supported by regional three-dimensional modeling. Flow in the Rustler Fm. during the wet period of the late Pleistocene was probably driven by a higher water table than that of the present and probably followed the local topography from east to west at the WIPP, rather than northwest to southeast. Drier conditions of the Holocene resulted in less, but perhaps not zero, recharge, and the altitude of the water table fell. Flow directions in the Culebra shifted to their present north-to-south direction, reflecting regional topography of the Delaware basin.

Early assessments of system performance (e.g., DOE, 1980) did not consider the possibility that climatic change could affect the transport of radionuclides through its effects on ground-water flow. The 1991 preliminary performance assessment for the WIPP contained the first quantitative analysis of the possible effects of climatic change on radionuclide transport through the Culebra (WIPP Performance Assessment Division, 1991, p. 6-35 - 6-43). The effects were approximated by varying heads along a portion of the northern boundary of a two-dimensional flow model for the Culebra. Heads were varied using a function that resulted in three peaks during the next 10,000 years, separated by periods in which heads were lowered to their present values. The maximum head elevations were prescribed by a sampled parameter that, at its largest value, allowed heads to reach the land surface and resulted in the maximum potentiometric gradient across the domain.

The 1992 preliminary PA for the WIPP used an approach similar to that of the 1991 analyses (WIPP Performance Assessment Department, 1992, p. 6-11 - 6-19). Sensitivity analyses performed for both the 1991 and 1992 preliminary PAs indicated that cumulative radionuclide releases were not sensitive to the variation in heads at the northern boundary,

conditional on the other assumptions adopted in the preliminary performance assessments (Swift et al., 1994, p. 9-12).

Variations in boundary heads were abandoned for the Compliance Certification Application because the regional three-dimensional modeling provided the basis for an approach that was better linked to the near-surface processes of infiltration and recharge and that offered more control over ground-water flow within the controlled area. The degree to which variations in boundary heads affected flow over the repository in previous analyses was in part determined by the location of the boundaries and their distance from the site. Setting boundary conditions closer to the repository could have had a greater effect on flow over the site. Furthermore, restricting changes in boundary heads to a single location restricted the possibility for changes in flow direction.

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9. Information Supporting Model Choice And Confirmation

See the attached memorandum:

Corbet, T.F., and P.N. Swift. 1996. "Records Package: Non-Salado Parameters Required for SECOFL2D: Climate Index," memorandum to NWM Records Center dated April 24, 1996, Albuquerque, NM: Sandia National Laboratories.

10. Validity and Completeness Interface/Integration with PA and Computational Models

In addition to work performed to address the treatment of climatic change in the Compliance Certification Application (see memorandum attached for Section 9), additional work was performed using the regional three-dimensional ground-water model to examine the validity of approximating three-dimensional flow in the Rustler with a two-dimensional model of the Culebra. This work indicates that within the controlled area essentially all flow out of the Culebra is lateral. This result, documented in FEP NS-9, provides the basis for applying a scaling factor derived from a three-dimensional model to a two-dimensional model.

Repository and
Salado Initial and
Boundary Conditions

1. Model Name

Repository and Salado Initial and Boundary Conditions.

2. Responsible Contact

P. Vaughn.

3. Model Description and References

Several important concepts are used to determine the initial conditions of the disposal system. There is no evidence of significant natural fluid flow in the Salado Fm. over time periods of regulatory interest. This is interpreted for the purposes of a conceptual model to mean that there is no natural flow in the Salado. It has been observed that Salado pore pressures in relatively undisturbed rock are elevated above hydrostatic from the surface but below lithostatic. Far-field pore pressures are thought to be near lithostatic. Small quantities of gas have been observed flowing to boreholes from the Salado, presumably due to exsolution from brine as pressure drops, but, because this has been investigated separately and found to be insignificant, the Salado is conceptualized as containing no gas initially. Because the excavation would be open for many years prior to decommissioning, the initial conditions for long-term performance near the repository are conceptualized as having been affected by brine flow toward the excavation, formation of a DRZ, and depressurization.

The conceptual model for the boundary conditions of the Salado model (in other words, the effect of the unmodeled Salado on the modeled Salado) is that there is no interaction between the unmodeled Salado and the modeled Salado. To ensure that this assumption does not affect results of the modeling, the boundaries of the model are placed more than 20 km from the regulatory boundaries of interest.

The initial state of the repository for evaluating long-term performance is based on the simplifying concept that some of the important processes leading to repository closure, which in reality occur over several years, all occur at the same time, and that some processes that in reality begin as soon as excavations are created do not begin until the repository is sealed:
- creep closure has not occurred (i.e., the initial volume equals the design excavation volume);
- waste has just been emplaced and has not degraded or interacted in any way in the repository;
- shaft seals and panel closures have just been emplaced;
- the repository, having been just sealed off, has atmospheric pressure; and
- the repository contains no more liquid in the emplaced waste than the limits prescribed by the WAC.

As mentioned above, the important concept that several years of open excavations affects the pressure, saturation, and rock properties in the Salado is included.

4. Model Purpose

Initial conditions describe the effects of events and processes occurring prior to the start of simulations of long-term performance on the disposal system. Boundary conditions describe the interaction between the environment excluded from the model and processes included in the model during the simulation of long-term performance.

5. Principal Parameters and Relationship among Parameters Defined by the Model

The principal parameters generally called initial and boundary conditions are those that are solved for in the mathematical model of processes, such as pressure, saturation, and flux. However, in the most general sense, all parameters must be specified at the beginning of a simulation and all parameters are specified along the boundaries of the model domain, even though at that location most of them would be meaningless. The following sections describe the initial and boundary conditions specified for the two-phase flow code, BRAGFLO, used in this performance assessment. Initial values of parameters not discussed in the following sections are set equal to the values assigned from the performance assessment database or LHS sampling that are discussed elsewhere.

Disposal System Flow Modeling (BRAGFLO). In BRAGFLO, initial conditions for the simulation of the regulatory period are consistent with the following:
- there are no gradients for flow in the far-field Salado;
- Salado far-field pore pressures are above hydrostatic from the surface but below lithostatic; and
- near the repository, excavation and waste emplacement results in partial drainage of the DRZ and subsequent evaporation of drained brine into mine air, followed by removal from the modeled system by air exchanged to the surface.

"Far-field" refers to the region that is not influenced by the drainage of the DRZ. For units above the Salado, initial pressures are set to be consistent with observed pore pressures or normal hydrostatic gradients.

Estimating the effects of DRZ drainage during the operational period is not simple. For each vector sampled in LHS, BRAGFLO simulates a period of time representing disposal operations. This calculation is called the start-up simulation and covers five years, from $t = -5$ years to $t = 0$ years, corresponding to the amount of time a typical panel is expected to be open during disposal operations. Most of the initial parameters used during the regulatory period simulation ($t = 0$ to $t = 10,000$ years) are also assigned for the start-up simulations, with some exceptions that are described below.

The initial pressures in the Salado for the start-up simulation are calculated based on a sampled pressure in MB 139 at the shaft and adjusted throughout the Salado and the DRZ to account for changes in hydraulic head due to changes in altitude. This adjustment assumes hydrostatic equilibrium. The DRZ permeability is set at 10^{-17} m^2 for the start-up simulation. Based on observed changes in the DRZ, the DRZ porosity is adjusted upward 0.0029 (0.29%)

from the sampled value for intact impure halite. Initial pressure for the start-up simulation in the excavated regions is set to atmospheric. The shaft is modeled as unfilled, with the same physical properties as the excavation.

For the start-up simulation, an initial water-table surface is specified within the Dewey Lake Red Beds at an altitude of 980 m. This altitude is consistent with field observations. Above the water table, pressure is maintained at one atmosphere, 0.101 MPa; liquid saturations in these cells are held constant at residual liquid saturation. Below the water table, initial liquid saturations in all regions except the repository and shaft are 100%. Pressures are set consistent with a hydrostatic gradient below the water table within the Dewey Lake and the Rustler Fm. except for the Magenta and Culebra. An initial pressure for the Culebra is set at 0.822 MPa, consistent with observations. An initial pressure of 0.917 MPa is specified for the Magenta, consistent with observations. Even though the natural properties of the units above the Salado vary considerably over the domain modeled by BRAGFLO, the BRAGFLO initial condition of constant pressure and constant properties for each layer is considered reasonable because the purpose of the BRAGFLO calculation with respect to these units is to calculate the flux of brine from the borehole or shaft to each unit or to the surface. For this purpose, the pressure and properties at the borehole or shaft are important, but details of regional hydraulic head and unit properties are not.

For the start-up simulation, permeabilities of all units above the Salado are set to zero so that flow cannot occur from these units into the shaft. This modeling assumption is adopted so results of the start-up simulation will be consistent with the existence of effective liners in the shafts during disposal operations.

For the start-up simulation, no-flow boundary conditions are assigned in the BRAGFLO model of the disposal system along all of the exterior boundaries of the computational mesh except at the far field boundaries of the Culebra and Magenta and the top of the model (that is, the ground surface). These boundaries are 20 km from the boundary of the Land Withdrawal Area. The ground surface is maintained at atmospheric pressure. The boundaries of the Culebra and Magenta are maintained at pressures of 0.822 MPa and 0.917 MPa, respectively, corresponding to the initial pressure conditions used in the Culebra and Magenta. The pressure in the Castile brine reservoir is set at its sampled value for the start-up simulation.

During the start-up simulation, fluid flow calculated by BRAGFLO from the Salado and the DRZ into the excavated region simulates the effect of drainage into the repository during the operational period. Following the completion of the start-up simulations, initial conditions are specified for the regulatory period simulation. Boundary conditions for the regulatory period simulation are the same as those for the start-up simulation.

The regulatory period simulation begins with conditions specified consistent with the sealing of the repository by construction of shaft seals. Certain properties assigned for the start-up simulation are changed to make model conditions consistent with the emplacement of waste and completion of sealing. The liquid saturation in the waste-disposal region of the repository is set at a value consistent with the liquid saturation of emplaced waste, and other areas of the

excavation are assigned zero liquid saturation (100% gas saturation), regardless of the quantity of brine that may have flowed into the excavation during the start-up simulations. This is consistent with the observed ability of circulating mine air to remove any inflowing brine by evaporation. The entire repository is assigned an initial pressure of one atmosphere. Pressures and saturations in model regions representing rock remain as they were calculated to be at the end of the start-up simulation. Permeabilities of the units above the Salado are reset to the values specified for them. The shaft is assigned properties for shaft seal materials. The pressure in the shaft is set to one atmosphere, and the liquid saturation of shaft materials is set to 1.0 except in asphalt, where liquid saturation is zero. Waste is emplaced in the waste-disposal regions at a concentration of 163 kg/m^3 for ferrous metals and 65.2 kg/m^3 for biodegradable materials, and other waste properties are assigned. Panel closure properties are assigned to the panel closure regions. Permeability in the DRZ is raised to 10^{-15} m^2; this value remains constant for the regulatory period simulation. Corrosion and biodegradation reactions that produce gas are modeled to begin at the start of the regulatory period simulation, and their rates depend on the sampled parameter values for the gas generation model and the availability of brine.

Initial and Boundary
Conditions for the
Culebra

1. Model Name

Conceptual model for initial and boundary conditions used in two-dimensional modeling of ground-water and transport flow in the Culebra Dolomite Member of the Rustler Fm.

2. Responsible Contacts

J. Ramsey.

3. Model Description and References

Simulations of ground-water flow and transport in the Culebra require specification of initial conditions that define the initial state of the system to be modeled and boundary conditions that specify behavior at the limits of the model domain.

Culebra Boundary Conditions. Ground-water flow in the Culebra is computed at regional and local scales. The purpose of the regional simulation is to incorporate natural flow boundaries into the problem domain that may influence the magnitude and direction of flow in the region of interest. Regional scale simulations are performed over a large problem domain using a relatively coarse computational grid. The results of the regional scale simulations are used to interpolate boundary conditions at the local scale. This modeling approach allows the use of high resolution computational grids in the region of interest with the incorporation of natural flow boundaries at a much larger scale.

The regional domain (Figure 4) is ~22 by 30 km and aligned with the axis of Nash Draw along a portion of the western boundary. Nash Draw is a highly conductive discharge region that behaves hydraulically as a ground-water divide (see Section 2.2.1.1). Therefore, the portion of the western boundary oriented along Nash Draw is represented by a no-flow boundary. The remaining regional boundary conditions are essentially unknown. When possible, they are positioned to align with topographic highs or other geologic features, such as San Simon Swale on the northern boundary. Due to their uncertainty, the boundaries are positioned far from the local problem domain to reduce the influence of the boundary conditions on the solution in the region of interest. Because boundary head values can be easily computed from existing well data, Dirichlet (constant head) boundary conditions are used on these boundaries.

The WIPP land withdrawal boundary, local grid domain, and waste panel area are superimposed on the regional grid in Figure 4. The placement of boundaries in the local domain were selected to capture important flow paths and facilitate the computation of integrated release across the land withdrawal boundary. The results of previous performance assessments, in conjunction with preliminary test simulations, indicate that the dominant ground-water flow pattern is south to southwest. To maximize problem resolution and minimize computational requirements, a portion of the land withdrawal boundary in the northern section is excluded from the local grid. Therefore, the local domain encompasses most of the land withdrawal boundary and extends slightly beyond its southern and western borders.
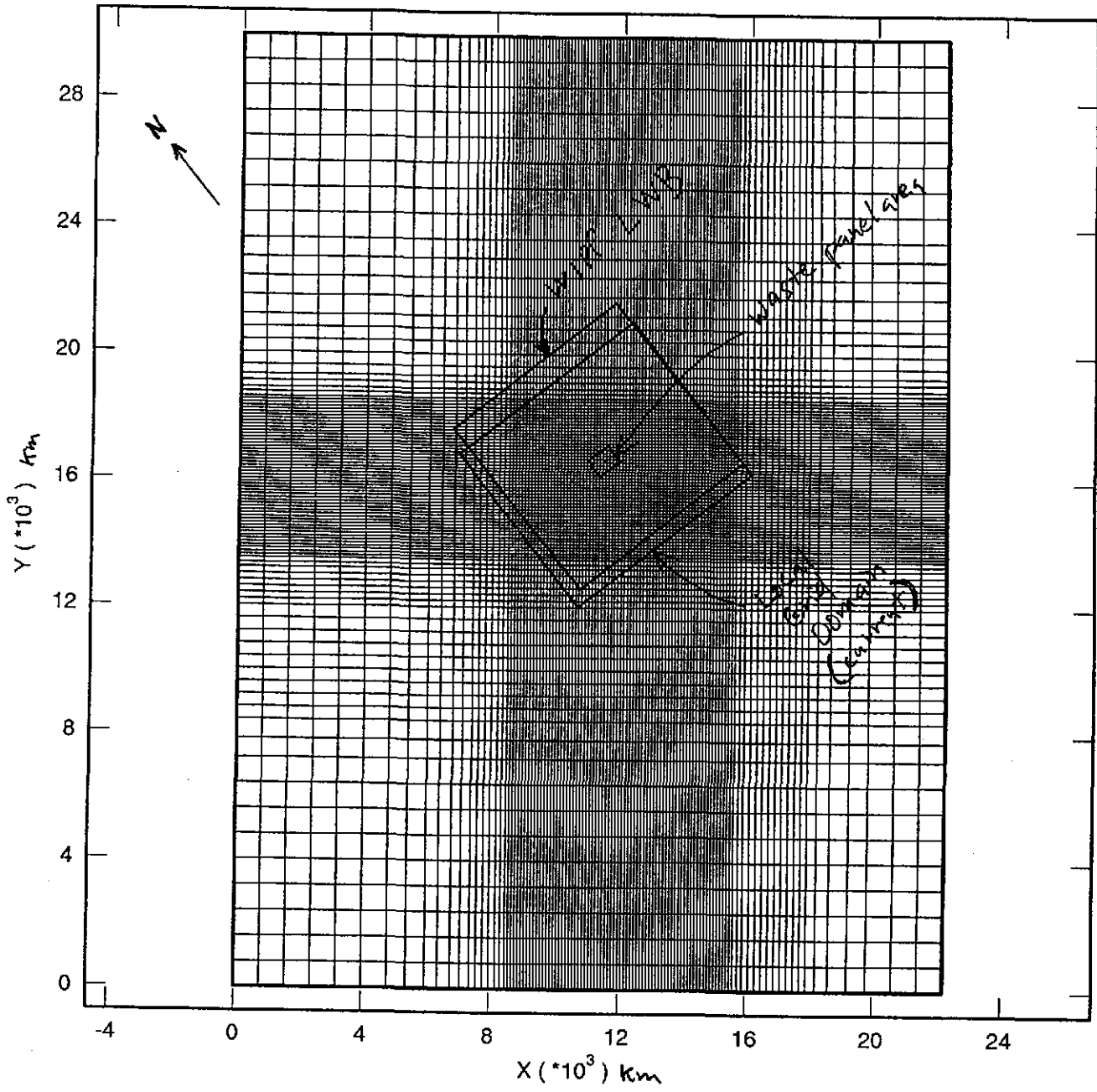
Figure 4. Regional grid.

The computational grid of the local domain is shown in Figure 5. The local domain is ~7 by 7 km. The grid contains 75 columns and 65 rows resulting in 4875 grid blocks.

Boundary conditions of the local domain were arbitrarily chosen to be Dirichlet and derived by interpolating the solution of the regional domain. Because these simulations are steady state, specification of the boundary condition as Dirichlet or Neuman will produce essentially identical results.

Culebra Initial Conditions. An initial estimate of the undisturbed head distribution is required to analyze transient well data needed to generate the transmissivity fields. These data were obtained from hydrographs of the WIPP boreholes measured prior to the excavation of the first shaft. The hydrographs depict a quasi-steady state flow field for 10 to 20 years preceding shaft excavations.

Initial conditions for the Culebra flow and transport calculations are trivial. Spatial head distribution is provided in the flow simulation only as an initial guess of the steady state solution. Initial actinide concentrations in the transport simulations are assumed to be zero.
References:

Initial and boundary conditions for SECOFL2D and SECOTP2D used in the Compliance Certification Application are described in Section 6.4.10.2 and Appendix TFIELD.

4. Model Purpose

Initial and boundary conditions are chosen to provide a reasonable and realistic basis for two-dimensional simulations of ground-water flow and transport to be used in estimating radionuclide transport through the Culebra.

5. Principal Parameters and Relationship among Parameters Defined by the Model

Initial conditions must be specified for all primary solution variables used in a transient analysis. Freshwater head is the primary solution variable in the codes for ground-water flow (SECOFL2D) and transmissivity field generation (GRASP-INV). Isotope concentration is the primary solution variable for the ground-water transport code (SECOTP2D).

Initial values of freshwater head are required at each grid block location by GRASP-INV to analyze transient well data. Initial values of freshwater head are also required by SECOFL2D. However, because ground-water flow will be simulated assuming steady-state conditions, the initial head provided to SECOFL2D only serves as an initial guess of the steady-state solution. Finally, the initial concentration of each isotope transported is required by SECOTP2D.

The potential boundary conditions that can be imposed by the above simulators are specified head/concentration, specified flux, or mixed boundary conditions (a combination of the two).
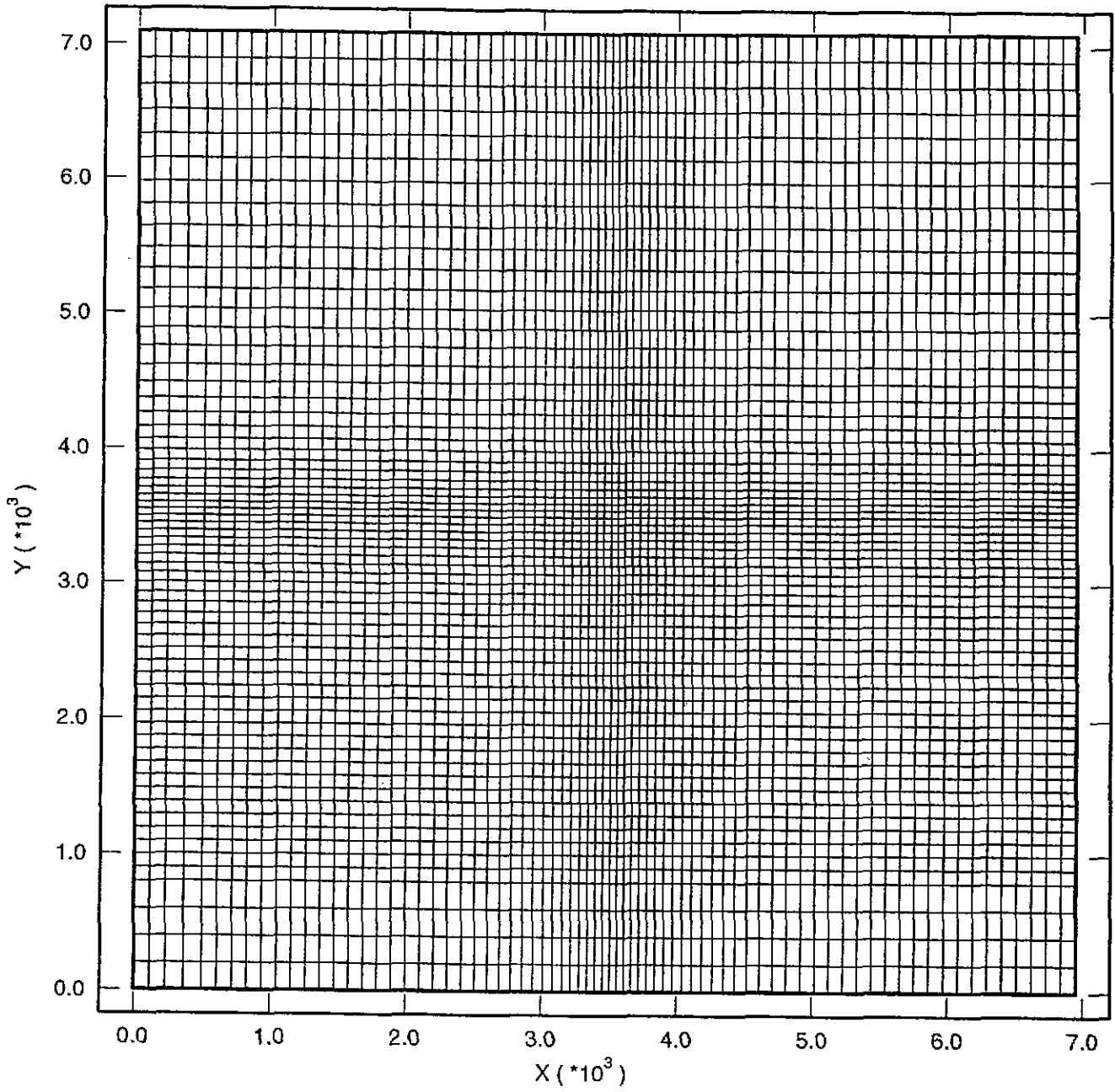
Figure 5. Local grid.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Initial Conditions. The undisturbed freshwater heads used by GRASP-INV are derived from hydrographs of the WIPP boreholes measured prior to the excavation of the first shaft. These hydrographs depict a quasi-steady state flow field for periods of 10 to 20 years preceding shaft excavation. Although some uncertainty exists about this parameter, the effect of this uncertainty is believed to be insignificant relative to the effect and associated uncertainty of climatic variations and potash mining on flow and transport.

Boundary Conditions. Other than Nash Draw, the regional boundary conditions are essentially unknown. Due to their uncertainty, these boundaries are positioned far from the local domain to reduce their influence on the solution in the region of interest. This uncertainty is also thought to be relatively insignificant when compared to the influence and uncertainty of climate variations and potash mining.

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

See "Culebra," Section 8.

9. Information Supporting Model Choice and Confirmation

See "Culebra," Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models.

See "Culebra," Section 8.

Colloidal Actinide
Transport in the
Culebra

1. Model Name

Colloidal Actinide Transport in the Culebra.

2. Principal Investigator for Model or Components

H. Papenguth.

3. Model Description and References

Colloidal particles in moving ground water may be affected by a variety of processes, such as advection, diffusion and dispersion, interactions with pore walls, sorption, filtration, and disintegration. For each colloidal particle type included in WIPP performance analyses, the processes of advection in the bulk fluid flow and only one retardation process are conceptualized. This simplification prevents the undesirable complication of the numerical modeling methods.

Colloidal particles in moving ground water travel faster than the average velocity of small dissolved molecules. This fact is included in the conceptual model. Because these effects are inherently captured by the experiments that have been executed to characterize colloidal retardation processes, the model parameters developed from these experiments included these effects.

The concepts of advective porosity and diffusive porosity discussed in the dissolved actinide transport conceptual model are also important in the colloidal actinide transport model. All colloidal particles are transported in the advective porosity. Some colloidal particles are small enough to diffuse into the diffusive porosity and sorb there. Each colloid is assumed to respond to certain processes, and each is discussed separately.

Microbes are relatively large colloidal particles. They are too large to participate in diffusion and cannot enter low permeability regions of the Culebra. It is thought that they will be transported in advective porosity and retarded only by filtration. Filtration strains large colloidal particles from moving ground water as it passes through regions of the advective porosity that have apertures small enough to block microbes. For implementation as a mathematical model, filtration is assumed to behave analogously to a decay process.

Mineral fragments are also relatively large colloidal particles. Their transport behavior is conceptualized and modeled analogously to microbes; however, different filtration parameters are applied based on experimental results.

Humics are colloidal particles small enough to diffuse from advective porosity into diffusive porosity, and therefore they behave similarly to dissolved actinides, although with different parameter values. The processes that act on humic colloids are advection, diffusion and dispersion in the advective porosity, diffusion into diffusional porosity, and sorption within the diffusional porosity. Filtration and sorption with fracture walls are not included in the conceptual model.

The intrinsic colloid formed by Pu(+4) (the Pu polymer), the only actinide-intrinsic colloidal particle stable at WIPP, is small and behaves analogously to humics, although with different parameter values.

4. Model Purpose

The purpose of this model is to represent the effects of colloidal actinide transport in the Culebra.

5. Principal Parameters and Relationship among Parameters Defined by the Model

Transport parameters of diffusion coefficients and dispersivities are required for all colloidal particles because these processes occur in advective porosity. The principal retardation parameters for microbes and mineral fragments are the decay constants, which are used to treat the process of filtration. Humics and the Pu(+4) polymer require tortuosity and sorption parameters (K_ds).

Transport of colloidal particles in the Culebra Dolomite is coupled to several other conceptual models. An important coupling is to features that can introduce colloids to the Culebra, e.g., the exploration borehole, shafts and shaft seals, and colloidal actinide source term. The most important coupling is to the model for flow in the Culebra. Because transport in the Culebra is one of the last processes to occur along this pathway prior to potential release, it does not feed back on other conceptual models in any significant manner. In a manner of speaking, this conceptual model falls at the downstream end of the overall disposal system model, and thus has limited impact on those models that come before it.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

After introduction of colloidal actinides and dissolved actinides into the Culebra, realistically a new equilibrium condition will be established, with the stipulation that the total concentration of actinide must be preserved. Several components participate in establishing a new equilibrium:

- actinides precipitated or coprecipitated with carbonate or sulfate salts resulting from the mixing of repository and Culebra brines;
- dissolved actinide ions and complexes with anthropogenic organic ligands introduced from the repository;
- actinide polyelectrolyte macromolecules (i.e., the immature actinide intrinsic colloid or polymer) from the repository;
- actinides sorbed onto mobile colloidal sorbing substrates (e.g., humic substances) from the repository;
- actinides sorbed onto mobile colloidal sorbing substrates (e.g., humic substances) present in Culebra brines;
- sorption of dissolved actinides or complexes onto the Culebra host rock; and
- cosorption of colloidal actinides onto the Culebra host rock.

As in the repository, quantifying an equilibrium assemblage is beyond the Project's capabilities. Consequently, the Project has elected not to attempt to link processes.

The effect of naturally occurring colloidal particles in the Culebra is included in the source term by supplementing the repository's colloidal actinide source term with the potential contribution from Culebra colloidal particles. A more obvious approach would have been to modify the repository source term as it was introduced to the Culebra, perhaps by assigning a portion of the dissolved actinide to the concentration of naturally occurring colloidal particles in the Culebra. That approach is not consistent with the implementation of SECO-TP, however, as is seen in the following example. In a particular time step within a PA realization, a mass of actinides is introduced into the nodal block in the Culebra intersected by the intrusion borehole and immediately mixed with the contents of that nodal block. The impact of naturally occurring colloidal particles in the Culebra must be defined by the mass of actinides that may sorb to those particles, which is therefore specified as a mass per unit volume (i.e., concentration) term. In the event that colloidal particles are not retarded, the two colloidal source terms may be added at the Culebra without introducing artifacts. If, however, colloidal actinides are retarded, then the concentration of colloidal actinides in that nodal block continually increases with subsequent time steps as Culebra colloidal particles are added. Supplementing the repository source term avoids that artifact, although the approach is probably overly conservative.

Mineral-fragment colloidal particles are unique among the four colloidal particle types addressed for WIPP, because their concentrations are not generally linked to solubility, as are actinide intrinsic colloids and humic substances, or to a maximum supportable population in the case of microbes. Consequently, in an intrusion scenario at the WIPP, as dissolved actinide elements are introduced to the Culebra, it is possible that those dissolved actinides could sorb onto a separate population of indigenous mineral fragments, producing a supplemental source term. To account for that possibility, the geometric mean value was multiplied by a factor of two.

In its current implementation, SECO-TP allows four types of retardation:
- retardation within matrix porosity accessed by advective flow, following a matrix advection single-porosity conceptual model for hydrogeologic flow;
- retardation within matrix porosity accessed by diffusion, following a fracture advection-matrix diffusion double-porosity conceptual model for hydrogeologic flow;
- retardation within a thin layer (e.g., a clay-lining, see Papenguth and Behl, 1996b) adjacent to fracture surfaces; and
- retardation on a fracture surface.

A complication arises in the treatment of large-diameter colloidal particles such as microbes and large mineral-fragment colloids, because they are too large to diffuse into the matrix porosity. Instead, retardation of microbes will be simulated by filtration using a decay approach.

A complication associated with quantifying colloid-facilitated actinide transport (as well as transport and retardation of dissolved actinide species) is that the heterogeneous properties of the Culebra must be considered. Ground-water composition in the Culebra is variable, especially

when considering an intrusion scenario that introduces Salado and Castile Formation brines. The rock fabric of the Culebra, both locally and regionally, is also variable, and may affect hydrogeologic flow. That variability of physical and chemical properties along a potential flow path cannot be measured directly. Several types of rock fabric have been observed in core collected from the air intake shaft and elsewhere (Papenguth and Behl, 1996b).

8. History of Model Development and Alternatives Considered and Rejected

Colloid-facilitated transport of actinides has not been included in past performance assessment calculations because of the lack of adequate information to model this phenomenon and demonstrate its impact on compliance (see, e.g., WIPP PA Department, 1992a, p. 4-12, line 29). Transport of actinides by colloidal particles has been recognized only relatively recently as a phenomenon of critical importance to the performance of nuclear waste repositories (Jacquier, 1991; Avogadro and de Marsily, 1984). In fact, the study of colloid-facilitated contaminant transport is a relatively new topic to the geosciences in general. Concern about the potential for accelerated radionuclide transport due to sorption on colloidal sized particles began in a study of a liquid waste disposal site in Los Alamos, New Mexico (Nyhan et al., 1985). Since then, a number of researchers have investigated colloids as a potential transport mechanism (e.g., McCarthy and Zachara, 1989; Corapcioglu and Jiang, 1993; Grindrod, 1993; Ibaraki and Sudicky, 1995). Grindrod (1993) and Ibaraki and Sudicky (1995) addressed the topic of colloid-facilitated transport through fractured porous media, and their work is therefore the most applicable to the Culebra Dolomite. Neglecting a major difference in conceptualizing the interaction between colloids and dissolved isotopes, the conceptual model discussed here is nearly identical to that of Ibaraki and Sudicky (1995). Each of these authors consider colloids to be a third phase that can sorb contaminants in a manner similar to the immobile solid phase. In their models, the concentration of a contaminant sorbed to a colloid is expressed as some function of the dissolved contaminant concentration. Therefore, to solve the colloid-facilitated transport problem, these authors simultaneously solve mass balance equations for the colloid and the contaminate. This is a very rigorous approach that requires the development of specialized numerical models to solve.

To avoid developing an additional transport code specifically to model colloid-facilitated transport, the Project elected to make a number of simplifying assumptions under the presumption they are conservative with respect to the integrated release of radionuclides. The first assumption is that the dissolved concentration will be greatest at the source point and therefore, the concentration of radionuclides sorbed to colloids will be greatest at the source as well. Second, a radionuclide sorbed to a colloid is assumed to remain fixed to that colloid throughout the simulation. Given these assumptions, the isotope concentration sorbed to colloids is no longer a function of the dissolved isotope concentration, and it is not necessary to solve the dissolved species transport problem simultaneously with the colloid transport problem. As a result, the standard advection diffusion transport equation can be used to predict colloid transport and compute integrated colloid releases. Given the initial concentration of radionuclides sorbed to each specific type of colloid, the integrated colloid release can be converted to an integrated isotope release by postprocessing the colloid transport results. Isotope decay can also be accounted for in postprocessing.

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9. Information Supporting Model Choice and Confirmation

Three approaches could be used to quantify colloid-facilitated actinide transport at the WIPP. First, the transport of one or more types of actinide-bearing colloidal particles in the Culebra could be assumed to be instantaneous. In other words, as actinides associated with that type of colloidal particle migrate to the Culebra from the repository, or are generated within the Culebra, the mass of actinides associated with those colloidal particles becomes part of the

integrated release of actinides at the accessible environment boundary. This approach can be useful if the concentrations of actinides associated with one or more types of colloidal particles is very low. Treating colloid-facilitated actinide transport as instantaneous, however, is a significant shortcoming, because of the potentially large expected retardation effects of colloidal particles.

Second, the existing advection-dispersion numerical code (SECO-TP; Roache, 1993) and supporting codes could be used to simulate the effects of one or more of the colloid retardation phenomena. The dual porosity advection diffusion equation solved by SECOTP2D can simulate colloid sorption in the matrix and to the fracture walls. The code can also model colloid filtration using the decay term of the governing equation. For colloids considered too large to diffuse into the matrix, matrix diffusion can be disabled by setting the matrix tortuosity to zero. This approach was used for some calculations completed in 1994. Specifically, microbes, because of their relatively large size, were excluded from matrix diffusion and limited to advective flow in fractures. Humic substances were allowed to diffuse into intercrystalline pores, but at a reduced rate relative to dissolved actinide species. This numerical simulation approach has been used by other organizations in performance assessments of other sites.

Third, colloid-facilitated actinide transport could be quantified by a rigorous numerical modeling code developed for the WIPP. Such a rigorous transport model would address all physical and chemical processes that could affect the movement and fate of the four colloidal particle types, including colloid generation; interactions with solutes, the dispersant, and rock; advection; dispersion; diffusion; filtration; gravitational settling; attachment and detachment; adsorption and desorption; coagulation; flocculation; peptization, etc. Ideally, permeability reduction due to pore clogging by colloids, which would affect solute transport as well, would also be considered. Currently available models do not include all the processes.

Among the most sophisticated rigorous numerical models are those being developed by van der Lee et al. (1993, 1994) and Bennett et al. (1993). Many of the colloid transport numerical models described in the literature focus on simulating solute transport through fractured media with double porosity flow characteristics, and they have been generalized to include unique features of colloid transport (e.g., Hwang et al., 1989; Grindrod and Worth, 1990; Light et al., 1990; Smith and Delgueldre, 1993; Harmand and Sardin, 1994). Some numerical models, such as the population balance model by Travis and Nuttall (1985), assume equilibrium colloid concentrations. That is, the loss of colloidal particles by attachment to the medium wall is compensated by the generation of new colloidal particles by various mechanisms such as condensation and entrainment ("simultaneous birth and death"). The modeling approach developed by Travis and Nuttall (1985), however, is similar to the dual-porosity transport model equation.

None of the rigorous numerical codes was designed for long-term performance assessment calculations like those required for the WIPP Project. One way to simplify the numerical modeling is to isolate complicated mechanisms from the colloid-facilitated contaminant transport numerical models. For evaluation of the performance of the WIPP, this has been done by quantifying kinetic stability outside any transport model. The remaining phenomena can be

treated empirically. A significant reduction in the potential effect of colloidal particles on the performance of the WIPP can be made at the source term level, without consideration of the transport properties of those colloidal particles.

The most practical approach to evaluating the transport of colloidal actinides is the second option presented above, use of the existing SECOTP2D numerical code (Roache, 1993). Where possible, the Project will reduce the number of phenomena that must be treated in the transport code and address them in the source term. For example, the effect of ionic strength on colloid stability will be included in the colloid source term. Retardation of colloidal particles will be quantified using a retardation factor or through a decay term.

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10. Validity and Completeness Interface/Integration with PA and Computational Models

Transport of colloidal actinides has been numerically simulated using a advective-dispersion code that is designed to quantify transport of dissolved species. An adequate simulation of colloid retardation can be conducted by simplifying quantification of colloid retardation so that only one retardation mechanism is considered for each colloid type. Microbe and mineral-fragment retardation is described by a filtration approach. Humic and Pu(+4)-polymer retardation is described by more conventional chemical retardation (K_d) parameters.

Exploration
Borehole

1. Model Name

The Intrusion Borehole (long-term flow).

2. Responsible Contacts

Current practice: Bill Thompson (CTAC), Bill Coons (CTAC).
Implementation in PA codes: Palmer Vaughn and Jon Helton.

3. Model Description and References

Boreholes may intersect the repository during the next 10,000 years. Such boreholes would affect the containment properties of the disposal system in two principal ways. During drilling, actinides may be brought directly to the surface (see Section 6.4.7.1, Releases During Drilling). After the borehole has been plugged and abandoned, it remains as a potential conduit for fluid flow among the repository, overlying units, and the hypothetical Castile brine reservoir.

40 CFR 194 establishes that the properties assigned to the borehole for the long-term should be based on current practice for abandoning boreholes in the Delaware Basin (documented in a draft report in preparation, attached). Section 6.4.7 describes the properties assigned to the boreholes for performance assessment.

The conceptual model for long-term flow up a plugged and abandoned borehole addresses possible flow interactions among the Salado, the more permeable rock units above the Salado, the repository, and a Castile brine reservoir. The properties of the borehole may change with time, depending on the type of plugs emplaced. Long-term flow through the borehole may affect pressure and saturation in the repository by Darcy flow, hence affecting the direct releases associated with subsequent penetrations. No retardation of actinides or other transport-limiting effects in the borehole are assumed.

4. Model Purpose

The purpose of the intrusion borehole (long-term flow) model is to provide in BRAGFLO the physical properties relevant to fluid flow through a plugged and abandoned borehole that intersects the repository. The model includes several possible plug patterns because 40 CFR 194 requires the DOE to base its modeling on the currently used practices in the Delaware Basin when a borehole is plugged and abandoned; currently, several practices are followed.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The principal parameters in the intrusion borehole model for long-term flow are permeability, porosity, compressibility, and two-phase properties. Because these properties may change with time as the borehole plugs degrade, some types of boreholes have several defined stages for the evolution of borehole properties.

There is no direct correlation among the parameters in the model. Permeability, the most important borehole property, changes according to the stage of borehole development. The values assigned to other parameters are held constant for all stages and are set consistent with a borehole fill referred to as silty sand, consisting of the material that would naturally slough off the walls of the borehole or the remains of degraded plugs. The porosity of the plugged and abandoned borehole is set at a low value within the porosities expected of materials that will be in the borehole; the low value was chosen because smaller void volume in the borehole reduces storage in the borehole and slightly increases the total flux of fluids that may pass through it.

This conceptual model is related to several others. The long-term flow model for the intrusion borehole is not directly coupled to the models for direct release (Cuttings, Cavings, and Spallings and Direct Brine Flow); however, because the long-term properties of the borehole may allow the pressure and saturation in the repository to change, estimates of direct release may differ for a previously intruded repository and an undisturbed repository. This is accounted for in performance assessment. Long-term flow through the intrusion borehole is the only way in which a Castile brine reservoir may influence the containment properties of the disposal system (although this can influence the direct releases calculated for subsequent boreholes).

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Predictions of the time-dependent permeability of plugged boreholes are based on three configurations for borehole plugs and two concepts of how the plug materials will be altered by fluids. The plugging configurations and materials have been developed from reviews of current plugging operations as they are practiced in the Delaware Basin of New Mexico. The interaction of plug materials and fluids is modeled using traditional concepts from equilibrium thermodynamics with empirical and model-generated data relevant to alteration of plug materials.

Predictions of plug performance derived from the conceptual models are sensitive to both chemical and physical parameters. Key areas of uncertainty include the following:
- the "openness" of the physical and chemical systems;
- the initial porosity of the hardened concrete plug;
- the initial permeability of the hardened concrete plug;
- the degree to which performance data from generic materials applies to WIPP-specific materials and conditions;
- the conditions at the precise locations where WIPP plugs are emplaced; and
- the physical dimensions of the plugs.

Openness. The conceptual models for predicting the time-dependent permeability of plugged boreholes recognize two types of systems: open and closed. Open systems are ones in which components can be added or subtracted freely, whereas closed systems are ones in which the identity and amount of components available for reaction are constant. In physical models, a closed system maintains a constant volume, while in open systems volume is unconstrained. The principal area of uncertainty in the conceptual models is the definition of the boundary between open and closed space. This boundary is significant because real systems are somewhere between

totally open or closed, and open and closed systems result in very different expected performance lives for plugged boreholes.

In chemical systems, a very small addition or release of reacting components is insignificant, but a substantial change can have large effects: in open systems reactions proceed until the supply of reactants is exhausted. In open systems, equilibrium considerations may have little or no significance; hence treatment by equilibrium thermodynamics may be unenlightening. Similarly, in physical systems, a small amount of system expansion will have little effect on internal stresses, but unlimited expansion may cause the system to fail in tension.

Corrosion of the casing steel has been modeled thermodynamically for plugged boreholes. Hydrogen is a common byproduct of corrosion. An equilibrium hydrogen pressure has been calculated for a number of potential reactions, using metallic iron to represent steel and pure water to represent brines. Attainment of equilibrium hydrogen pressure is taken to indicate cessation of corrosion. To reach equilibrium, the system must contain the hydrogen that is generated. The hydrostatic pressure of the brine column has been assumed to confine hydrogen when the pressure exceeds the equilibrium hydrogen pressure calculated for the corrosion reaction of interest.

The reactions thought to be most representative of steel corrosion produce iron hydroxide corrosion products. Equilibrium hydrogen pressures for these reactions are exceeded by hydrostatic pressures at depths greater than about 1100 feet. Corrosion of casing above this depth is treated as open; the casing corrodes until the supply of metallic iron is exhausted and the casing disintegrates. Without axial support supplied by the casing, the concrete plug also fails. In contrast, corrosion is assumed to take place in a closed system at depths greater than 1100 feet. Hydrogen is not free to nucleate as a gas and leave the system. Although local perforations in the casing are expected, the casing does not disintegrate. It supports the concrete plugs, and permeability changes in the plugs are attributed to alteration of cement phases by the brine that flows through them.

Chemical alteration of cement phases by brine produces new solids with greater molar volumes than the unaltered, hardened cement phase. In a closed physical system, the alteration will lead to decreased internal porosity and consequent decrease in permeability. In an open physical system, alteration will lead to increased internal pore pressures that will eventually exceed the tensile strength of the concrete plug. The result is often seen on concrete sidewalks or other unreinforced concrete structures: without something to restrain expansion, the concrete cracks, increasing its porosity and permeability.

Current plugging practices create configurations that favor each model. Plugs installed to respond to the New Mexico Oil Conservation Department's (OCD's) regulation R-111-P approach 2000 feet in length. These plugs are judged to be long enough that they are self-confining. As a result, alteration of R-111-P plugs produces a situation in which performance is indistinguishable from the undisturbed rock. In contrast, plugs emplaced in response to regulations of the U.S. Bureau of Land Management have a mean length near 40 m. This length is judged to be too short to provide self-confinement; alteration of the concrete results in

fracturing and increased porosity and permeability in the plug. The plug length that changes the physical system from open to closed is undetermined. For both chemical and physical model elements, a closed system enhances performance.

Initial Concrete Plug Porosity and Permeability. Simulation of concrete plug degradation follows a model proposed by Berner (1990), in which the matrix degrades after dissolution and removal of soluble materials such as alkali salts. The model is grounded in empirical observations that concrete alteration sequentially removes excess alkalis, portlandite, and tobermorite or CSH. Decreased strength attends removal of portlandite.

A critical amount of flow must occur before this degradation threshold is crossed. A volume equivalent to 100 pore volumes has been taken as the critical flow volume, based on values for common compositions of ordinary portland cement concrete (OPC) (Berner, 1990). Also following Berner, the model tracks the amount of flow as pore volumes, reasoning that flow occurs only through pores and that alteration is therefore limited to the solids that surround the pores. The model does not explicitly account for the strength of the concrete but instead makes the conservative assumption that physical failure occurs suddenly at the onset of chemical attack on CSH, i.e., at ~100 pore volumes. As a result, initial porosity of the hardened concrete is a key parameter for timing plug degradation.

The initial permeability of hardened cement is directly related to the connected porosity that permits flow to occur. Initial permeability of OPC is a strong function of the water:cement ratio of the mix. Higher water contents produce higher porosity and permeability. To simplify the analysis, initial plug permeability has been taken as a constant at 5×10^{-17} m^2. This value lies in the upper range of permeabilities reported for OPC and is verified by field measurements made during a single field test of borehole plugging conducted for the WIPP Project.

The initial permeability of the concrete plug is an important parameter because water must penetrate and flow through the structure before it can alter the hardened plug. The lower the permeability, the longer it takes for 100 pore volumes to pass through the plug. Somewhat paradoxically, the lower the porosity, the smaller the volume of water needed before attack of the CSH begins, because the model decouples the relationship between porosity and permeability by holding permeability constant. In the real world, cement formulations with low water:cement ratios generally produce fewer alkalis and have both lower porosities and lower permeabilities. Less water must pass through the concrete body before onset of CSH degradation, but the lower permeabilities lead to a longer life. The simplified model is conservative: it holds the permeability constant at the upper end of the established range while allowing porosity to vary over the full range commonly encountered in OPC. This accommodation reflects better knowledge of permeabilities than porosities in as-emplaced borehole plugs. The range in porosity modeled (5% to 40%) can create an order-of-magnitude spread in predicted performance life.

Generic Data Base For Performance Properties. The only quantitative performance data for borehole plugs near WIPP are hydraulic measurements that were made as part of field demonstrations. Qualitative data have been produced by recovery, microscopic inspection, and leach testing of concrete cores recovered from nearby potash mines. These data establish that

plugs placed in boreholes will have low initial permeabilities and that plugs placed in the Salado will form tight interfaces at the borehole-rock interface and will not degrade substantially by contact with formation brines in the amounts and compositions that might reasonably be expected.

From the outside inward, the conceptual model for borehole plugs envisions concentric circles of OPC (grout attaching the casing to the rock), low carbon steel (the casing), and a central disc of OPC (the concrete plug). The bulk of the data used to predict the service lives of borehole plugs comes from the open literature on corrosion of low carbon steel and OPC and from tabulated thermodynamic data bases.

There are many low-carbon-steel alloys, and not all corrode at the same rate in a given environment. However, because of the aggressive corrosion rate selected for the model, steel composition is not thought to introduce significant uncertainty about the rate. The cementitious materials used in hydrocarbon exploration are also variable. The degree to which oil-field materials might perform differently from the cement mixtures investigated and reported in the literature is unknown. There is no standard mix formulation that specifies plugging cements precisely; the use of generic data is reasonable, because the vagaries of cement composition are implicitly included. The published empirical studies of concrete degradation include a large body of data for reacting solutions ranging from pure water to marine brines. Waters with higher chloride and magnesium contents cause greater reaction. This level of detail has not been factored into the model directly; rather, alteration by brines has been the favored source when extracting information on degradation.

The greatest uncertainty associated with composition is likely to arise from the thermo-dynamic calculations used in the model. Pure phases (Fe for steel and H_2O for brine) have been assumed so that hand calculations may be more readily performed. Various reactions and environments have been modeled without directly considering complexities in the chemical system (other than volatiles). Qualitatively, the added complexities are likely to have no substantial consequence on the ability of the brines to dissolve a pathway through the casing. However, system complexities might decrease the equilibrium hydrogen pressures calculated for the corrosion reactions or lead to unexpected reaction products.

Location and Dimensions of Plugs. The conceptual models for borehole plugs examine three basic possibilities: a continuous plug through the evaporite sequence, a plug below the brine reservoir horizon coupled with a plug between the repository and the Rustler, and three or more plugs with at least one intermediate plug between the brine reservoir and the repository and another between the repository and the Rustler. These possibilities represent simplifications of the plugging schemes documented in the 1996 survey. In the conceptual model, all plugs are taken to be 40 m long.

The basis for these assumptions is a detailed survey of plugging practices in the Delaware Basin. The locations of plugs are determined partly by stratigraphic changes and partly by operational considerations during exploration and recovery. Variations in plug length and location affect pressure regimes and flow rates through plugs. The 40-m length of the plugs is the approximate mean value of ~188 plugs in the survey. Minimum lengths prescribed by regulations

are 50 feet above plus 50 feet below casing transitions or recovery points. Additional plug lengths sometimes occur for unspecified reasons. When all else is equal, performance life is proportional to plug length. For conservatism, the model does not consider the longer plugs.

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

The borehole permeability model was assembled beginning in February 1996. Initially, the model considered only the plug configuration stipulated by OCD regulations, but it was subsequently expanded to consider all regulations and practices documented in the New Mexico portion of the Delaware Basin, without specific consideration of their applicability to WIPP in the future.

From its outset, the model included elements for evaluating steel corrosion and concrete degradation. Initially, thermodynamic equilibrium was assumed for all situations. This approach was subsequently rejected for shallow systems in light of the reasoning that hydrogen evolved by corrosion probably would not be constrained indefinitely within the confines of the borehole plug and casing.

The model was developed to be straightforward and easy to understand. Use of hand calculations was favored over the use of complex computer codes. As a result, no detailed evaluation of potentially applicable codes was undertaken, and no screening of codes (or submodels) accepted and rejected was compiled.

9. Information Supporting Model Choice and Confirmation

The text of the report describing the model and its predictions contains about 40 references containing data that support the model. In general, these references support the plug configurations, steel corrosion mechanisms and rates, and concrete alteration processes that underpin the model.

The plug configurations are based on a detailed survey of plugging practices documented in the Delaware Basin of New Mexico. The data base contains information on ~188 boreholes, which is the entire record of boreholes constructed since 1988, when modern plugging practices began. The survey examined the lengths, locations, and intervals plugged, as well as the materials used for construction.

Data supporting low-carbon-steel corrosion models come primarily from the literature. The empirical data support the assumption that general corrosion is the dominant mechanism for corrosion under oxic conditions and that pitting will occur under low oxygen (and high pH) or elevated carbon dioxide/hydrogen disulfide conditions. Corrosion rates are a function of the conditions under which corrosion occurs. Published data include rates as rapid as 3 mm/yr, which

is the value assumed in the model. Such rapid rates are not inconsistent with reports in the Delaware Basin of casing failures occurring from corrosion within months to years. Data from corrosion of steel enshrouded in concrete come from the literature on marine construction and the data base on reinforcing steels. These data support the assumption that steel encased in concrete cannot be assumed to corrode more slowly than exposed steel.

Data supporting the concrete degradation model come primarily from two sources: the international repository literature and journals on concrete construction (e.g., dams or bridges). The international literature on repositories contains both models and empirical studies confirming that alteration of concrete will result in decreased porosities and permeabilities in closed systems. Experience for dams confirms this conclusion and confirms the diffusion-driven concrete alteration rates used in the model. The general concrete literature has been used to establish likely ranges of the initial permeability and porosity of hardened concrete. Observations on WIPP field-emplaced borehole plugs confirm that use of the upper end of generic permeabilities is appropriate (5×10^{-17} m^2). Observations made on cores recovered from potash mines near WIPP confirm that alteration of concrete plugs is not extensive after decades of service.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See Section 6 above and Section 6.4.7.2 of the CCA.

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Direct Brine
Release

1. Model Name

Conceptual model for BRAGFLO direct-brine-release calculations.

2. Responsible Contact

Daniel M. Stoelzel.

3. Model Description and References

Direct brine releases may occur when a future driller penetrates the WIPP and unknowingly brings contaminated brine to the surface during drilling. (These releases are not accounted for in the cuttings, cavings and spallings calculations, which models only the solids removed during drilling.)

Certain conditions must exist within the waste for contaminated brine to flow directly to the surface during a drilling intrusion. First, pressure in the waste must be greater than that exerted by the column of drilling mud that penetrates a waste panel. Drillers in the Delaware Basin currently use salt-saturated mud with a specific gravity of 1.23 while drilling through the Salado. This corresponds to ~8.0 x 10^6 Pa at the repository horizon, which is the minimum pressure needed to move repository fluids upward in the well bore in the presence of a static column of drilling mud. Second, mobile brine must be present in the waste panels. Corrosion and biodegradation consume brine and release gas as a by-product, and it is possible for the brine volume in the waste pores to drop below the point of saturation. Gas-only flows up the drill hole may occur (see Cuttings, Cavings, and Spallings).

Prior to BRAGFLO direct-brine-release calculations, a procedure will be developed to adequately represent the variation in time and space of a wide range of drilling intrusions with a minimum number of direct-brine-release calculations. Specifically, a series of times and locations within the excavated waste area will be used to define the initial and boundary conditions from each 10,000-year consequence calculation for the direct release model.

4. Model Purpose

This model provides a series of calculations to support the Direct Brine Release portion of the 1996 performance assessment of the WIPP repository site. These calculations will support the complimentary cumulative distribution function (CCDF), the probability distribution of exceeding normalized cumulative radionuclide releases to the accessible environment, that will become part of the CCA.

5. Principal Parameters and Relationships Among Parameters Defined By Model

The pressure and saturation time-histories for each of 1500 realizations from the 10,000-year BRAGFLO calculations will provide the basic input needed for the direct brine release calculations. The pressure and saturation at specified times for each consequence calculation will

provide the initial and boundary conditions for a separate repository-scale BRAGFLO model to determine the direct release to the surface.

The input parameters used for the direct-brine-release calculations come from four sources: the 10,000-year BRAGFLO output files, the CUTTINGS_S code, the WIPP database, and a correlation to simulate flow up the borehole. The initial brine saturation and pressure, porosity, and crushed panel height used in the direct-release model are determined from the 10,000-year BRAGFLO results, and therefore vary with time. These parameters are calculated by time interpolation in the CUTTINGS_S code and relayed to the direct-release model. Unsampled material properties that remain constant are read directly from the parameters database (through MATSET). Sampled material properties are taken from the 10,000-year BRAGFLO output. The pressure (boundary condition) that drives the BRAGFLO wellbore model has been developed from a commonly used petroleum industry multi-phase vertical pipe flow correlation, which is tied to the well deliverability expression used by BRAGFLO. This "flowing bottom-hole pressure" depends on an assumed wellbore geometry, brine saturation, and pressure within the intruded panel for each realization.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Uncertainty in the BRAGFLO direct-brine-release calculations is captured in the 10,000-year BRAGFLO calculations from which the initial and boundary conditions are derived. The model parameters that have the most influence on the direct brine releases are repository pressure and brine saturation at time of intrusion. Brine saturation is influenced by many factors, including Salado and marker bed permeability and gas-generation rates (for undisturbed calculations). For E1 and E2 intrusions, Castile brine-pocket pressure and volume and abandoned borehole permeabilities influence conditions for the second and subsequent intrusions. Dip in the repository (hence the location of intrusions), two-phase flow parameters (residual brine and gas saturation, etc.), time of intrusion, and duration of flow have lesser impacts on brine releases.

7. FEPs Associated with Model Development

DR-4, Circulation of Fluid in Repository up a Borehole to the Surface.
DR-5, Recirculation of Castile Brine through Waste and to the Surface During Drilling.

8. History of Model Development and Alternatives Considered and Rejected

Originally, a simplistic cylindrical (radial) BRAGFLO model was used to represent the excavated volume of one intruded panel, but this was inadequate to capture the effects of heterogeneities within the site. This model was replaced with the current repository-scale mesh representing the proposed eight-panel configuration of the WIPP excavation, accounting for drifts, passageways, seals, pillars and rooms, and formation dip in the waste region. This mesh was further refined to evaluate the effects of sub-panel seals (room scale) and other engineered barriers on the flow behavior through the system, which influenced direct releases. The current mesh reflects the latest configuration proposed by DOE (panel seals only), with flow unaffected by backfill within the panels, which is similar to the original repository-scale model. In addition,

the vertical wellbore flow model is coupled to the BRAGFLO mesh, and the effects of solids removal caused by cavings and spall are examined (CUTTINGS_S code). Boundary conditions can account for two intrusions in a single panel, one of which connects to a brine pocket.

Most of this recent work is as yet undocumented. Reports will be provided throughout the CCA process as model results are produced.

9. Information Supporting Model Choice and Confirmation

The assumptions used in the models are based on current drilling practices in the WIPP area of the Delaware Basin. The wellbore model description assumes a typical WIPP-area oil well completion, including bit size, casing size and depths, drilling mud, etc. The duration of flow is based on how a present-day driller might react to the pressures and flows predicted by the model when encountering a high-pressure panel. The assumptions in the BRAGFLO direct-brine-release model (i.e., about permeability, two-phase flow properties, crushed panel height, porosity, etc.) match those used in the 10,000-year BRAGFLO and CUTTINGS_S models.

10. Validity and Completeness Interface/Integration with PA and Computational Models

The WIPP two-phase flow code BRAGFLO is used to simulate the direct brine releases during a drilling intrusion. This code is also used to calculate the 10,000-year flow of brine and gas through the WIPP and surrounding rock. However, a different conceptual model has been constructed to represent the excavated rooms, drift passageways, and the salt pillars between them. This refined mesh, or "repository scale" model, more accurately captures the flow patterns associated with the short-duration direct releases. The suite of software used to calculate direct brine releases is shown in Figure 6. The output from the repository-scale direct release model is the volume of brine (m^3) released to the surface.
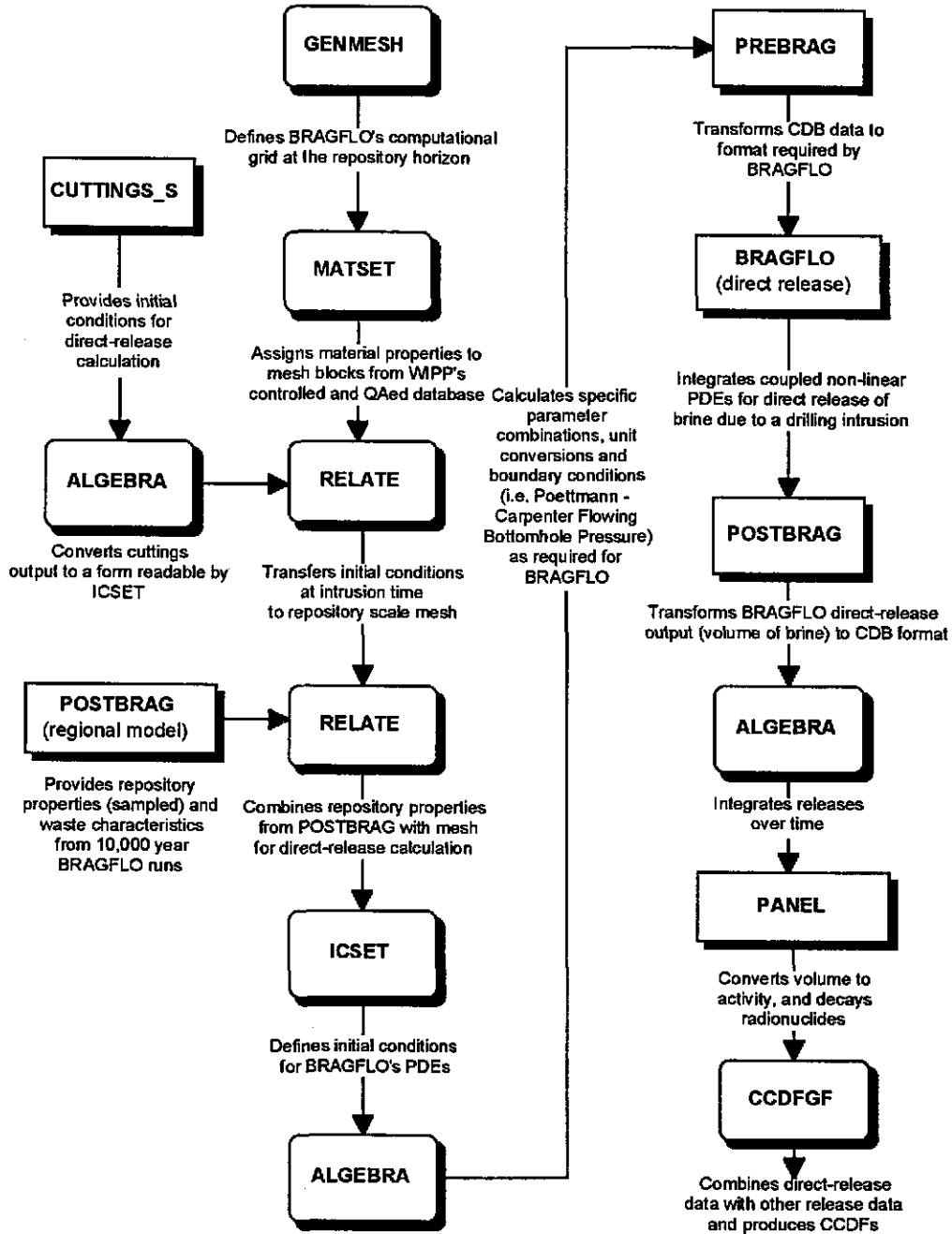
Figure 6. The code sequence for the BRAGFLO direct-release
calculations in the 1996 CCA performance assessment.

Cuttings, Cavings,
and Spallings

1. Model Name

Direct Releases: Cuttings, Cavings, and Spallings.

2. Responsible Contact

Barry Butcher.

3. Model Description and References

The conceptual model for cuttings, cavings, and spallings is discussed in three parts because of the differing process by which the three types of material are produced.

Cuttings are materials removed to the surface through drilling mud by the direct mechanical action of the drill bit. The volume of waste removed to the surface is a function of the compacted repository height, the porosity of waste at the time of intrusion, and the drill bit area. The radioactivity of waste removed to the surface is probabilistically determined based on the distribution of waste radioactivity expected in the WIPP.

Cavings are materials introduced into the drilling mud by the erosive action of circulating drilling fluid on the waste in the walls of the borehole annulus. Erosion is driven solely by the shearing action of the drilling fluid (or mud) as it moves up the borehole annulus. Shearing may be caused by either laminar or turbulent flow. Repository pressure effects on cavings, which are negligible, are covered by the spall process.

Spallings are the particulate material introduced into drilling mud by the movement of gas from the waste into the borehole annulus. After the drill bit enters the repository, pressure gradients generated by the flow of gas toward the borehole fracture the waste material, permitting the escaping gas to flow within fractures rather than through a porous matrix. Consequently, the intrinsic permeability of the matrix does not restrict gas flow, and the gas pressure at the borehole entrance to the repository can be assumed to be the initial gas pressure in the repository. The gas flow velocity up the borehole is governed by the isothermal flow of gas in a long tube of a given cross-sectional area, tube roughness, and gas pressure at the borehole entrance. The mass-flow rate of gas in the fractured waste at any radial cross-section is equal to the mass-flow rate up the borehole. Radial gas flow within the fractures in the waste matrix erode and widen the fractures. Erosion is assumed to occur if the fracture gas velocity exceeds a threshold velocity related to the terminal velocity of a waste particle at the fracture surface and to the cohesive strength afforded by moisture in the matrix.

4. Model Purpose

The purpose of these models is to estimate the quantity of actinides released directly to the surface during drilling through the repository by three mechanisms: the drillbit boring through the waste (cuttings), the drilling fluid eroding the walls of the borehole (cavings), and gas movement forcing particulate matter into the circulating drilling fluid (spallings).

5. Principal Parameters and Relationships among Parameters Defined by the Model

The cuttings model has as a principal parameter the diameter of the drill bit, which according to current practice is constant. This model interacts with the conditions in the repository as calculated by BRAGFLO because the porosity and height of the repository is necessary to calculate the volume of waste removed.

The principal parameters in the cavings model are the properties of the drilling mud, drilling rates, and the shear resistance of the waste.

The principal parameters in the spallings model are the gas pressure in the repository when it is penetrated and properties of the waste such as particle diameters and erosive properties. Because the release associated with spalling is sensitive to gas pressure in the repository, it is strongly coupled to the BRAGFLO-calculated conditions in the repository at the time of penetration. In particular, the spall release may be sensitive to whether the repository has been penetrated previously by another borehole.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Several factors contribute to model uncertainty, principally the undefined nature and complexity of the waste, both in its initial state and during its alteration by chemical and biological processes. Even the most basic information is lacking, such as chemical form, grain size (if the material is granular), partially biodegraded decomposed form, density, cohesion, etc. In the absence of such information, property values typical of surrogate materials are selected to represent the worst case response to the process being investigated. In this sense the model is highly conservative.

Another uncertainty arises from the drilling scenario assumptions for application of the model. There is no consensus about how the driller will act as the drill approaches the waste horizon, i.e., whether he will be able anticipate the presence of the gas-filled repository, much less control it once penetration occurs. In consequence, the conceptual model for the CCA assumes the worst possible situation, in which the borehole is driven almost instantaneously through the waste by a driller without any knowledge of the existence of the repository, and the driller is unable to control the subsequent gas release.

The scale-up from a model qualified on laboratory samples to the full-scale configuration of a drill penetrating the waste gives rise to another uncertainty. However, the adverse effect of improper scaling on the amount of waste released is considered to be negligible because of the extreme conservatism of the material and drilling scenario assumptions, in the sense that more release might actually occur than is predicted.

7. FEPs Associated with Model Development

See Appendix CUTTINGS.

8. History of Model Development and Alternatives Considered and Rejected

Waste can arrive at the ground surface as the result of the inadvertent penetration of the repository by an exploratory drill bit in three forms:

- cuttings - waste contained in the cylindrical volume created by the cutting action of the drill bit passing through the waste,
- cavings - waste that erodes from the borehole wall in response to the upward-flowing drilling fluid within the annulus, and
- spallings - waste introduced into the drilling fluid caused by the release of waste-generated gas escaping to the lower-pressure borehole.

The processes that produce these three forms of waste differ, and they can influence the quantity of waste transported.

Releases of cuttings and cavings are straightforward and have been consider in performance analyses since the beginning of cuttings release evaluation. The analytical equations governing erosion (cavings) based on laminar and turbulent flow (Berglund, 1992, Section 2.2) have been implemented in the PA code called CUTTINGS_S (WIPP PA User's Manual for CUTTINGS_S, Appendix A). Using appropriately selected input based on assumed physical properties of the waste and other drilling parameters, this code calculates the final caved diameter of the borehole that passes through the waste. Although certain features of the analysis, such as whether the flow of the drilling fluid should be modeled as laminar or turbulent and what drilling parameters might be valid near the WIPP repository, have been debated, the basic model has been generally accepted. The amount of material predicted to be released by cavings is small, and therefore this contribution to surface release has never been considered to be critical.

The conceptual model of the release of waste by spalling has been changed several times during its development. Early spall conceptual model development focused on transient unrestrained outgasing leading to the spall (dynamic fracture) of porous cohesive granular media (Berglund, 1992, Section 3.3). An experimental program related to model development focused on almost instantaneous depressurization and was limited to a one-dimensional linear sample configuration. The pore pressures required to cause spall or dynamic fracture could be closely approximated using the tensile strength of the porous soil medium (Berglund and Lenke, 1995), but the model was complex and could not be directly related to an intrusion event. In addition, although the experimental observations showed fracturing under instantaneous release of gas pressure, sample-preparation factors were largely responsible for the locations of the fractures. The fracture patterns also depended on the one-dimensional nature of the experiments, and the model did not explain how the fractured material was removed.

After extensive discussion, the dynamic fracture model was replaced with a more general three-part model based on the premise that the waste could be removed by any one of three mechanisms: blowout, stuck pipe, and gas-flow assisted erosion (as the result of gas-induced spall) (Butcher et al., 1994, Chapter 4). Which mechanism will dominate depends on the permeability and pressure drop at the borehole. Well blowout, an uncontrolled gas release from the well, was considered the dominant mechanism. The two remaining two mechanisms, stuck pipe and gas-flow assisted erosion, were not thought to be important because they would occur at waste permeabilities of less than 10^{-16} m^2

(Butcher et al., 1994, Sections 4.2.4.2, 4.2.4.3), much lower than is expected for the waste $(1.7 \times 10^{-13} \text{ m}^2)$. Consequently, conceptual-model development has focused on the blowout mechanism for removing waste.

Blowout models. Once the Project concluded that blowout was the principal cause of direct release of waste by spalling, the nature of the gas flow and the entrainment properties of the waste became the focus of subsequent model development. The first model, used in analyses in 1994 (Butcher et al., 1995, Section 4.2.4.1), was simplistic. Release was defined in this model by how much gas flowed out into the borehole and an assumed amount of solids entrained in it over a prescribed time period. The time limit for release assumed in the calculations was 5 minutes, the time estimated for the driller to close the blowout preventers and start weighting up the drilling mud. Entrainment was a sampled percentage ranging from 0 to 10%. Defending the time limit for release was particularly difficult because opinions about how long control of the well would take varied widely. Some wells are known to have required days or months to resume drilling. In addition, the model was not self-limiting, in the sense that release would continue for as long as the unchecked gas flow was assumed to continue, and quantification of the entrainment percentage was of concern.

To respond to these concerns, model development for release continued. A more-detailed model was developed based on the observation that a critical entrainment or lofting (terminal) velocity represents a threshold erosion condition. This value of the gas velocity defines whether solid particulate matter is separated from the bulk waste. Once separated, the material is assumed to be entrained in the gas and carried up the borehole to the ground surface (Berglund and Lenke, 1995, Section 6.1, pp. 33-39). Because gas velocities below this threshold can remove no solids, the removal process is self-limiting: gas velocity decreases as a function of distance from the borehole, eventually dropping below the entrainment velocity threshold and terminating the process.

The first version of the steady-state model incorporating the terminal velocity release process assumed that gas would flow uniformly through the waste and out the borehole. It was based on the fact that the velocity of the gas decreases with distance from the borehole, because of the symmetry of the gas flow field. The flow velocity is greatest at the borehole boundary and decreases with distance away from it. Therefore, at some point sufficiently remote from the borehole, the gas velocity just equals the critical entrainment (terminal) velocity. All material closer to the borehole was assumed to be eroded and lofted up the borehole, but the gas velocity in all material farther from the borehole was too low to cause erosion. This hypothesis permitted a calculation of how much material would be released in connection with an assumed gas-pressure drop in the waste.

An experimental program was designed to confirm the model using a test apparatus to simulate gas flow through the waste and up the borehole (Lenke and Berglund, 1995). In these tests, gas at a controlled flow rate was introduced into the circumference of a horizontal disk of material representing the waste, ~4 inches high and 20 inches in diameter, confined within a cylindrical vessel. Gas flowed through the sample and up through a tube (the borehole) vented to the atmosphere at the center of the top of the container. Solid material ejected from the tube, corresponding to a given value of gas pressure applied at the sample circumference, was weighed to determine its volume. A separate test determined the terminal lofting velocity for the sample materials as a function of particle-size distribution. Uniform vertical gas flow through a sample of material was increased until material was

"lofted" out of the container. Different terminal velocities were associated with different particle diameters.

The model-confirmation process was to first experimentally determine the entrainment velocity characteristics of the material, and then apply these data to the model to predict the amount of release expected for various boundary pressures. Boundary pressures were then experimentally applied to the samples in the experimental blowout device, and the amounts of eroded material were determined assuming uniform Darcy flow. The confirmation criterion was that if the measured amount of lofted material was less than the predicted amount of erosion then the model was considered confirmed. Confirmation was never possible, however, because the material release tests revealed that the assumption of uniform gas flow through the waste was not reflected by the response of the material. Instead of formation and expansion of a cavity left behind by eroded material, post-test observations showed that the gas instead created flow channels that increased in thickness as erosion proceeded. Releases were greater than expected because gas velocity in the channels was greater than it would have been had gas flowed through the bulk of the material (Lenke and Berglund, 1995, p. 14). Channel flow was consistent with the heterogeneity of the waste.

The experimental observation of flow-channels formation by erosion forced another iteration in blowout-model development to make the model consistent with material response. The new model (WIPP PA User's Manual for CUTTINGS_S, Appendix A, Section 2.3.1.3), called the channel flow model, is the one used for CCA calculations.

Including a channel-flow mechanism in the model requires either precise definition of the number, geometric configuration, and location of all the channels before they form, which is not technically feasible, or scaling the model results in some manner to reflect the channeling process. The scaling method was adopted, adjusting the predicted releases to agree with experimental release observations. Although the uniform-flow model was independent of experiments, in the sense that release predictions did not require direct data from the tests, a coupling between experimental results and the model was necessary for scaling. This was accomplished by introducing certain experimentally determined scaling constants into the model (Lenke et. al, 1996, p. 10 (in draft)). In spite of the presence of these scaling factors, the model is based on well-defined physical processes and is applied to different gases and solid materials by prescribing well-defined material properties, such as particle size and density, viscosity, and cementation tensile strength. The scaling factors are the only parameters of the model not directly related to geometry or material properties, but they are necessary to represent the way channels for gas flow are likely to develop.

9. Information Supporting Model Choice and Confirmation

See Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models

The cuttings conceptual model is implemented directly in numerical and computational models contained in the PA CUTTINGS_S code (WIPP PA User's Manual for CUTTINGS_S, Appendix A).

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WIPP PA User's Manual for CUTTINGS_S, Appendix A, Section 2.3.1.3, WPO# 36688, Version 5.00, March 25, 1996

Castile Formation
and Brine
Reservoir

1. Model Name

Conceptual model for the Castile Fm. and a hypothetical brine reservoir within it beneath the repository.

2. Responsible Contacts

Geoff Freeze, Kurt Larson, Al Lappin.

3. Model Description and References

The Castile Fm. is treated as an impermeable unit in performance assessment and plays no role in the analysis except to separate the Salado Fm. from the hypothetical brine reservoir that is important in human-intrusion scenarios. Properties of the hypothetical brine reservoir, including its permeability, porosity, volume, and initial pressure, are chosen to be consistent with available data from borehole penetrations of actual brine reservoirs in the region.

Basic geologic information about the Castile is given in Section 2.1.3.3. The hydrology of the known brine reservoirs is discussed in Section 2.2.1.2.2. The treatment of the brine reservoir in the performance assessment is discussed in Section 6.4.8.

4. Model Purpose

The conceptual model for the hypothetical brine reservoir is included in the performance assessment to estimate the extent to which uncertainty about the existence of an actual brine reservoir under the waste disposal region may contribute to uncertainty in the estimate of cumulative radionuclide releases from the disposal system. The conceptual model is not intended to provide a realistic approximation of an actual brine reservoir under the waste disposal region: data are insufficient to determine whether such a brine reservoir exists.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The principal parameters used in the brine reservoir model, described in Section 6.4.8, include permeability, porosity, pore compressibility, initial pressure, and two-phase flow properties. These parameters are implemented in the BRAGFLO model and affect the amount and rate of brine flow up an intrusion borehole. Brine flow up a borehole is also affected by conditions in other regions of the BRAGFLO model, including most directly the permeability of borehole-fill material and fluid pressure in the borehole. The volume of the brine reservoir, which is treated as an uncertain quantity in the performance assessment.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

Reeves et al. (1991) concluded that borehole transmissivity is the most important parameter in controlling flow from a Castile brine reservoir to the Culebra. Of the Castile reservoir properties varied in their analysis, the most important was initial pressure.

Performance assessment calculations in December 1992 concluded that repository performance was not sensitive to uncertainties in brine-reservoir properties over the sampled range of properties. However, long-term releases were sensitive to the presence or absence of a Castile reservoir. In other words, repository performance was sensitive to the scenario of a Castile reservoir being present, but not, within limits, to the detailed properties of this reservoir. The 1992 performance assessment also indicated that borehole permeability was a critically important parameter in repository performance, since a borehole is necessary to connect the Castile and repository with the land surface or Culebra Dolomite.

7. FEPs Associated with Model Development

There were no FEPs involving Castile brine reservoirs.

8. History of Model Development and Alternatives Considered and Rejected

The FEIS (DOE, 1980) acknowledged the possible importance of Castile brine, based largely on the encounter at ERDA-6. However, it concluded that brine probably was not present beneath the WIPP site, based on geologic structure and available well data (including the absence of brine in WIPP-12, prior to deepening). Scenario development for the FEIS considered brine occurrences, but consequences of a brine reservoir were not modeled explicitly. The presence of brine beneath the repository was considered to be extremely unlikely. No natural pathways connecting any brine reservoir with the repository were thought to be present. Boreholes penetrating the repository and any brine reservoir were assumed to be cased, and any flow from a reservoir would, therefore, have no impact (borehole-casing degradation was not considered).

Spiegler (1982) concluded that brine reservoirs, originally at hydrostatic pressure, formed several million years ago, prior to regional-scale erosion and decrease of overburden. He assumed an original connection of the reservoir to the water table and concluded that reservoirs formed (and were presumably isolated) several million years ago.

Spiegler and Updegraff (1983) concluded that the original brines were sea water, but that release of water from gypsum dehydration could not be ruled out. Popielak et al. (1983) agreed that Castile brines were relict or ancient sea water. They estimated a brine-residence time of about one million years, believing that isolation preceded the latest stage of basin tilting.

Faith, Spiegler, and Rehfeldt (1983), on the basis of analyses of brines from the WIPP-12 and ERDA-6 occurrences, concluded that these two reservoirs are isolated occurrences.

Lambert and Carter (1984), using several assumptions, calculated residence times for WIPP-12 and ERDA-6 ranging from ~25,000 to 880,000 years on the basis of U^{234}/U^{238} activity ratios. They concluded that there was a Pleistocene connection of the reservoirs to the Capitan Limestone, i.e., that the brines were originally fresh water.

By the time of the SPDV, Borns et al. (1983) concluded that
- reservoirs formed mainly due to gravity tectonics (in response to density inversion of thick halites and anhydrites);
- the WIPP-12 structure (1% strain) took a minimum of 10,000 years to form; and
- gravity tectonics were probably continuing, although at a reduced rate, due to decreased overburden over the past few million years.

The conceptual understanding of the origin of reservoirs did not change between the early 1980s and the time of the Draft and Final SEISs (DOE 1989, 1990). Brine reservoirs were (and still are) believed to be isolated occurrences. Based on a Time Domain ElectroMagnetic (TDEM) survey over the repository area, The Earth Science Technology Corporation (1988) estimated that a conductive horizon, which could be interpreted to represent Castile brine reservoirs, underlay portions of the waste-emplacement panels (4 out of 9 soundings directly over the panels).

For purposes of numerical modeling, hypothetical brine reservoirs were assumed to be radially symmetrical, with an inner highly-fractured zone of high transmissivity, and an outer (less-fractured) zone of moderate transmissivity. The outer zone is surrounded by an infinitely extending anhydrite matrix, representative of intact (unfractured) Castile. The brine-reservoir model produced double-porosity fluid-flow responses. This treatment implicitly assumes that any borehole intersecting an area underlain by a brine reservoir will produce large amounts of brine; the possibility that boreholes could penetrate the highly fractured reservoir, but miss highly conductive fractures, was not considered.

Assuming that the reservoirs are radial, and based on an areal views of wells penetrating the Castile (some of which did and some of which did not encounter a brine reservoir), Reeves et al. (1991) determined that brine reservoirs could be expected to have radii varying from ~800 to 3200 m. Deterministic calculations in the DSEIS and FSEIS assumed that any borehole penetrating the WIPP repository would penetrate a Castile brine reservoir, and that this reservoir could be represented by the estimated characteristics of the WIPP-12 brine reservoir.

There was no fundamental change in the conceptual understanding of brine reservoirs in the December 1992 performance assessment. PA calculations included gas pressurization of the repository, which was not considered in DSEIS calculations. This pressurization helped delay brine depressurization of the Castile reservoirs. It was estimated that brine underlay 25 to 57% of the waste-emplacement panels, with a median of 40%. This estimate was based on a contouring of the existing TDEM data, and was implemented as a probability of a given borehole intersecting brine. Any borehole penetrating a reservoir was assumed to produce brine. A broad range of significant reservoir properties (e.g., initial pressure, storativity) were sampled probabilistically, without assuming that any reservoir present would be represented by WIPP-12 properties. The WIPP-12 characteristics did, however, fall within the sampled range.

Section 6.4.8 of the CCA describes the WIPP Project's current model of a fractured Castile brine reservoir, as implemented by performance assessment. The main conceptual improvement is the realization that, due to the abundance of vertical fractures in Castile brine reservoirs, many boreholes may penetrate a brine occurrence without penetrating any conductive fracture. Therefore, although it is now assumed that a brine reservoir underlies the entire waste-emplacement-panel area, there is a reduced probability of a given borehole producing brine.

9. Information Supporting Model Choice and Confirmation

See Section 8.

10. Validity and Completeness Interface/Integration with PA and Computational Models

See Section 8.

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Multiple
Intrusions

1. Model Name

Multiple Intrusion Boreholes.

2. Responsible Contact

Jon Helton.

3. Model Description and References

If active and passive institutional controls fail, boreholes may be drilled in the future for resource exploration and development at the site. 40 CFR 191 and 194 require formal consideration of the possibility that active and passive controls will fail, and they regulate the period of time during which controls may be assumed to be effective in eliminating or reducing the probability of intrusion into the repository.

The conceptual model for intrusions is that they will occur randomly in time and space when active institutional controls are assumed to be ineffective, i.e., after 100 years according to the regulations. For a period of 700 years, the borehole intrusions are assumed to occur at a reduced rate, consistent with a study on the effectiveness of passive institutional controls and regulations. After 700 years, boreholes are assumed to be drilled on the site at a rate of $47/km^2$ per 10,000 years. The location and time interval between intrusions are determined probabilistically by a Poisson mathematical model. Because the repository is ~0.125 km^2 in area, in a group of randomly determined, hypothetical sequences of future events, the average number of boreholes intersecting the repository is about 6.

Because this conceptual model must be consistent with overall results of component models of the performance assessment modeling system, it uses insights gained from preliminary analysis, principally of BRAGFLO results, but also results from other codes. These insights will be documented in the CCA.

Two kinds of borehole intrusions are envisioned, called E1 and E2. Conceptually, E1 is a borehole that penetrates the repository and a Castile brine reservoir. E2 is a deep borehole that penetrates the repository without penetrating a brine reservoir. E1E2 is two or more boreholes intersecting a waste panel, at least one of which is an E1. For details on how these boreholes are used in scenarios, see Section 6.3.

Fluid flow through intrusion boreholes may affect the distribution of liquid and gas in the repository and the pressure in the repository. BRAGFLO calculations of disposal system performance with a single E1 borehole and with a single E2 borehole indicate that gas flows relatively freely between panels through panel closures and the DRZ around panel closures, but that liquid does not. Gas flow can equalize pressure throughout the repository.

Like the initial borehole, boreholes drilled after the first one may lead both to direct releases and to long-term releases. Reference conditions for direct releases are developed for initial

intrusions, for subsequent intrusions in the same panel, and for subsequent intrusions in a different panel, for several permutations of the large number of possible geometries.

Long-term releases to the Culebra Dolomite arising from subsequent boreholes are assumed either to be similar to releases from a single borehole or to be negligible, depending on the borehole combinations that are developed. For the E2 scenario, sequential E2 intrusions into the same panel are assumed to have no greater long-term consequences than one E2 intrusion. This is reasonable because the borehole is a high-permeability material in the disposal system. The flux through it is not limited by its properties, but rather by the rate at which liquid can enter the waste panels from the Salado Fm. An analogy for this behavior may be a piston in a hydraulic system: the rate of flow through the hydraulic pipes connecting the system depends not on the pipes' properties (borehole), but rather on the rate of movement of the piston (inflow from the Salado) and the expulsion of fluid from the piston chamber (the repository).

Because liquid flow between panels does not occur readily, the long-term releases associated with an E2 penetration of a previously unintruded panel are treated separately. For example, if each of two panels is intruded by an E2 borehole and no other, two E2 releases will be introduced into the Culebra. E1 intrusions into different panels are treated in the same way.

Any single panel penetrated by an E1 and at least one other borehole is considered an E1E2. Long-term releases from panels in which this occurs are calculated by the method described in Section 6.4.13.6.

4. Model Purpose

The conceptual model for multiple intrusion boreholes accounts for the effect on cumulative releases of multiple intrusions into the repository.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The principal parameter in the model is the rate at which boreholes are drilled. Previous intrusions have no effect on the location and timing of subsequent intrusions.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The timing and location of subsequent intrusions is determined probabilistically. The consequences of these randomly determined borehole locations and times are derived either from scaling results of similar calculations, or by scaling and simplification to less complicated results. Because separate calculations with all of the performance assessment codes are not performed for the combinations of future events that make up the CCDF, there is some uncertainty. The methods used to scale the releases from deterministic calculations are based on analysis of the behavior of the disposal system with defined sequences of future events and are considered reasonable simplifications.

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

The present methods for developing reference conditions for multiple intrusions strongly resemble the methods used in the 1992 preliminary performance assessment, although much in the model system has changed dramatically. The concepts and modeling techniques for this subject developed in the 1989, 1991, and 1992 preliminary performance assessments.

For the 1996 CCA performance assessment, an alternative to the method used for E1E2 intrusions was considered and rejected. This method was based on three assumptions about disposal system behavior during an E1E2 event:
- flow rates into the repository from the reservoir are constant or change slowly enough that they can be represented as constant for long periods of time;
- flow into the repository from the Salado or other sources during an E1E2 is negligible; and
- the repository becomes fully saturated soon after penetration of a Castile brine reservoir.

The alternative method would have used steady-state flow calculations between the Castile reservoir, the Salado, and the Culebra for any possible borehole configuration containing an E1 that occurs in the repository. This would have produced more realistic evaluations of the consequences of the E1E2 scenario; however, the assumptions it was based are not consistent with conditions observed in BRAGFLO disposal-system calculations. Because of the degradation of plugs in the boreholes, flow rates into the repository from the Castile do not change slowly. Flow into the repository from the Salado can be significant during an E1E2 occurrence. Finally, liquid does not flow readily through panel closures under most repository conditions, so the assumption of a fluid-saturated repository is not robust. Accordingly, this alternative method was abandoned, and the method described in Section 6.4.13.6, similar to past treatment, was adopted.

9. Information Supporting Model Choice and Confirmation

Information supporting the choice of the multiple intrusion model will be documented in the results section of the CCA and in sensitivity analysis documents.

10. Validity and Completeness Interface/Integration with PA and Computational Models

This conceptual model is based primarily on analysis of results of modeling done in this performance assessment completed prior to the final construction of CCDFs. Accordingly, it is well-integrated and consistent with the performance assessment as a whole and with the results of computational models in particular.

Mine Subsidence
Effects in the
Culebra

1. Model Name

Mine Subsidence Effects in the Culebra.

2. Responsible Contacts

Mike Wallace and Kurt Larson.

3. Model Description and References

See Section 6.4.6.2.3 of the CCA.

4. Model Purpose

This model incorporates the effects of potash mining in the McNutt Member of the Salado Fm. on disposal system performance into the performance assessment. 40 CFR 194 provides a conceptual model and parts of a mathematical model for these effects. The WIPP Project has implemented the EPA conceptual model to be consistent with EPA regulations and guidance.

5. Principal Parameters and Relationships among Parameters Defined by the Model

The principal parameter in this model is the range assigned to a factor by which hydraulic conductivity in the Culebra is increased. As allowed in supplementary information to 40 CFR 194, it is the only parameter that need be changed to account for the effects of mining.

Other parameters in the model, probably less important than hydraulic conductivity, are the extent of mining in the McNutt, the angle of draw above the mined areas, and whether and when potash mining occurs within the disposal system. The WIPP Project has developed its treatment of these parameters from 40 CFR 194 and its supplementary and background information.

6. Uncertainty in Conceptual Models and Relative Significance of Parameters

The EPA has provided the conceptual model for this process. The WIPP Project considers that any uncertainty associated with the conceptual model has been evaluated by the EPA and that the method specified is an acceptable representation of potential effects.

The most significant parameter in the model is considered to be the factor for multiplying hydraulic conductivity values in the Culebra transmissivity field. A second important parameter is the distribution of affected areas in the Culebra, for both the undisturbed mining case (mining outside the disposal system in the near future) and the disturbed mining case (mining within the disposal system in the future).

7. FEPs Associated with Model Development

None.

8. History of Model Development and Alternatives Considered and Rejected

Mining in the McNutt Member of the Salado Fm. has been considered in the performance of the WIPP since the original siting activities. Siting criteria for both the site abandoned in 1975 and the current site included setbacks from active mines. (See, for example, Historical Development.) The 1980 FEIS for the WIPP (DOE, 1980) considered the possibility of an indirect dose arising from the effects of solution mining for potash or halite; it concluded that direct access of waste by solution mining for potash was not likely because of the methods that would be used to control the flow of solvent through the formation. The Project is not aware of solution mining for potash or other minerals in the Salado Fm. within the Delaware Basin at this time.

Mining has been included in scenario development for the WIPP since the earliest work on this topic (e.g., Hunter, 1989; Marietta et al., 1989; Guzowski, 1990; Tierney, 1991; and Guzowski, 1991). These early scenario developments considered both solution and room-and-pillar mining. The focus was generally on effects of mining outside the disposal system. The two primary effects of mining considered were changes in the hydraulic conductivity of the Culebra or other units and changes in recharge as a result of surface subsidence. These mining effects were not formally incorporated into quantitative assessment of repository performance in preliminary performance assessments, but their inclusion in scenario development can be traced through the 1992 preliminary performance assessment.

The inclusion of mining in the CCA performance assessment satisfies the requirements of 40 CFR 194 to consider the effects of this activity on the disposal system.

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9. Information Supporting Model Choice and Confirmation

See 40 CFR Part 194, Supplementary Information and Background Information.

10. Validity and Completeness Interface/Integration with PA and Computational Models

The conceptual model and computational models for PA are well integrated; no portion of the conceptual model is omitted from the computational model, and nothing is incorporated in the computational model that is not also a stated part of the conceptual model.