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**Sandia National Laboratories
Waste Isolation Pilot Plant**

**Analysis Plan for Calculations of
Culebra Flow and Transport:
Compliance Recertification Application**

AP-100

**Task number
1.3.5.1.2.1**

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1. INTRODUCTION AND OBJECTIVES

In 1996, the Department of Energy (DOE) completed a performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the radiation protection regulations of 40 CFR 191 and 40 CFR 194. As required by the WIPP Land Withdrawal Act (Public Law 102-579), DOE is required to submit documentation to EPA for the recertification of the WIPP every five years following the first receipt of waste in order to continue operation of the site. This will require that a Compliance Recertification Application (CRA) be prepared and submitted to the EPA by March 26, 2004. The DOE expects to provide the CRA to the EPA during November 2003.

A new set of PA calculations will be included in the CRA submittal to EPA. Analysis Plan AP-105 (Leigh, 2003) presents the full set of PA calculations required for the CRA and lists the series of analysis plans that describe the specific details for each component model that will be run for the CRA. This analysis plan (AP-100) describes the set of calculations that will be run to simulate Culebra flow and transport in the vicinity of the repository for 10,000 years.

2. APPROACH

Culebra flow will be simulated using the MODFLOW/PEST suite of computer codes while Culebra transport will be simulated using the SECOTP2D computer code. The MODFLOW/PEST suite of computer codes is a replacement for the SECOFL2D suite of codes that was used to simulate Culebra flow in the CCA. The SECOTP2D code was used to simulate Culebra transport in the CCA.

2.1 CULEBRA FLOW CALCULATIONS

For the CRA, new Culebra transmissivity (T) fields are being created under Analysis Plan AP-088 (Beauheim, 2002a) using a different model domain, different gridding, different boundary conditions, and different codes from what were used for the CCA. The Culebra modeling domain for the CCA was an area approximately 22 km wide by 30 km long, with the long axis oriented northeast to southwest. A total of 10,800 grid blocks was used with dimensions ranging from 100 m to 800 m. The Culebra modeling domain for the CRA covers an area 22.4 km wide by 30.7 km long, but is oriented with the long axis north-south (Figure 1). A uniform grid of 68,768 100-m by 100-m blocks is being used for this model.

A combination of fixed-head and no-flow boundaries was used for both the CCA and CRA modeling, but the boundary conditions are different in each calculation. The northeast arm of Nash Draw was treated as a no-flow boundary (flow line) in both the CCA and CRA models. In the CRA model only, a no-flow boundary continues down the southeast arm of Nash Draw. As shown in Figure 1, cells in the CRA model domain that lie to the west of the no-flow boundaries in Nash Draw are inactive during model execution.

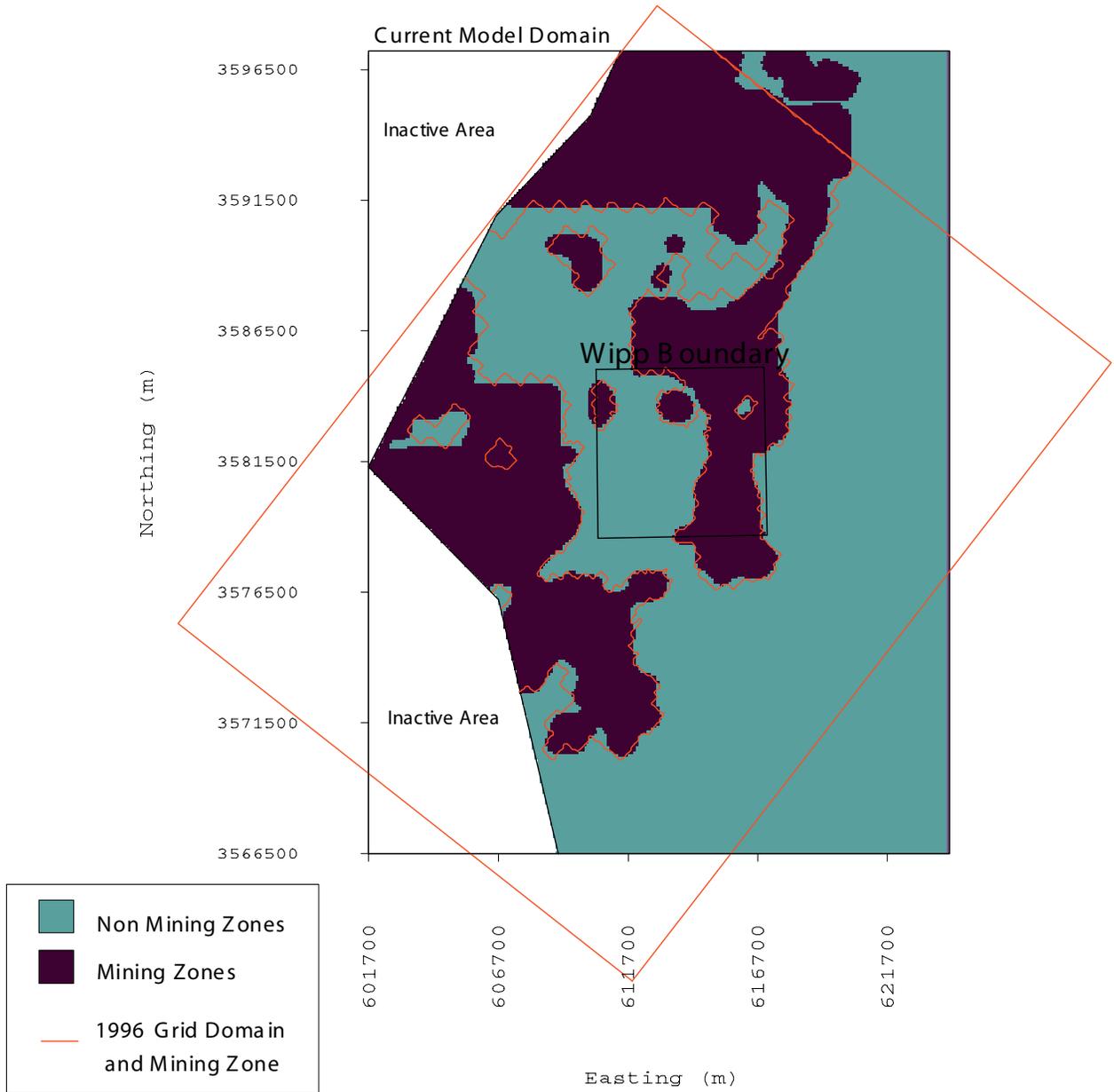


Figure 1. CCA and CRA model domains and mining areas.

Table 1. Comparison of CCA and CRA Freshwater Heads.

Well	CCA Freshwater Head (m amsl)	CRA (2000) Freshwater Head (m amsl)	Well	CCA Freshwater Head (m amsl)	CRA (2000) Freshwater Head (m amsl)
AEC-7	932.0	933.19	P-14	926.9	NA
CB-1	911.1	NA (not available)	P-15	917.8	NA
D-268	915.2	NA	P-17	909.3	915.20
DOE-1	914.3	916.55	WIPP-12	933.6	935.30
DOE-2	934.7	940.03	WIPP-13	933.7	935.17
ERDA-9	NU (not used)	921.59	WIPP-18	930.5	936.08
H-1	921.6	927.19	WIPP-19	NU	932.66
H-2b2	924.8	926.62	WIPP-21	NU	927.00
H-3b2	914.8	917.16	WIPP-22	NU	930.96
H-4b	911.4	915.55	WIPP-25	928.7	932.70
H-5b	934.2	936.26	WIPP-26	918.5	921.06
H-6b	932.0	934.20	WIPP-27	938.1	941.01
H-7b1	912.7	913.86	WIPP-28	937.5	NA
H-9b	906.4	911.57	WIPP-29	NU	905.36
H-10b	921.3	NA	WIPP-30	934.1	936.88
H-11b4	912.4	915.47	WQSP-1	NU	935.64
H-12	913.5	914.66	WQSP-2	NU	938.82
H-14	916.9	920.24	WQSP-3	NU	935.89
H-15	916.1	919.87	WQSP-4	NU	917.49
H-17	911.0	915.37	WQSP-5	NU	917.22
H-18	932.4	937.22	WQSP-6	NU	920.02
H-19b0	NU	917.13	USGS-1	909.8	NA

The Culebra flow calculations performed for the CCA and CRA differ in the head values used to define model boundary conditions, and in the value of transmissivity assigned at the H-3 hydropad. The head values used for the CCA were estimated from historic records (hydrographs) under the assumption that the Culebra was at steady-state prior to disturbances caused by WIPP activities. The CRA head values represent measurements made in late 2000, and are generally higher than the CCA values. The heads used for the CCA and CRA modeling are shown in Table 1 (Beauheim, 2002b).

Since the CCA was completed, the transmissivity of the Culebra at the H-3 hydropad has been revised based on additional interpretation of hydraulic tests (Beauheim, 2002c). The log 10 value of transmissivity used in the CCA was $-5.62 \text{ m}^2/\text{s}$. The revised value used for the CRA T fields is $-4.7 \text{ m}^2/\text{s}$.

2.2 MODIFICATION OF T-FIELDS FOR MINING

After the CRA T fields are calibrated to transient hydraulic-response data (Task 4 of AP-088), they are modified to account for the potential effects of future potash mining (Task 5 of AP-088). The mining modification is performed in two stages. The “partial-mining” modification is performed by increasing the transmissivity of the Culebra over areas that might be mined in the future outside the WIPP land-withdrawal boundary (“Mining Zones” in Figure 1). For each of the calibrated T fields, the Culebra T in the affected regions is increased by a random factor between 1 and 1000 produced by Latin Hypercube Sampling (LHS). For the “full-mining” modification, the T multiplier is applied to areas that might be mined both outside and within the WIPP land-withdrawal boundary. For a given T field, the same T multiplier is used for both the partial-mining and full-mining modifications.

The T fields used in the CCA were generated in SWIFT II with GRASP-INV controlling the calibration process. For the CRA, the T fields are being generated in MODFLOW-2000, using PEST v. 5.51 to guide the calibration process.

2.3 CULEBRA TRANSPORT CALCULATIONS

Radionuclide transport in the Culebra will be simulated using a two-dimensional dual-porosity or dual-continuum solute transport model to account for the fractured nature of the porous medium. The model assumes parallel-plate-type fracturing where fluid flow is restricted to the fractures (the advective continuum). Advection and hydrodynamic dispersion are considered to be the dominant physical transport processes within the fractures, while molecular diffusion is the dominant physical transport mechanism within the rock matrix (the diffusional continuum). The dual-porosity model includes diffusional mass transfer between the rock matrix and the fractures. Retardation is permitted in both the advective and diffusive continuum assuming a linear equilibrium sorption process. Radioactive decay is accounted for in the model through the use of multiple straight decay chains.

The Culebra radionuclide transport calculations will be performed using the SECOTP2D code. SECOTP2D is an implicit finite volume code that is second-order accurate in space and time. Advective terms are discretized using a Total Variation Diminishing (TVD) discretization scheme. Diffusion terms are treated using central differences. The time discretization is a generalized three-level scheme. SECOTP2D uses a staggered finite volume mesh in which the velocity components are defined at cell faces while concentrations are defined at cell centers.

The physical domain used in the transport calculations will be a subregion of that used for the groundwater flow calculations (Figure 2). This subregion will be approximately 7.5 km by 5.4 km, aligned with the principal directions of the groundwater flow domain. The transport domain will extend beyond the boundaries of the WIPP in the east-west direction (approximately 200 m in the west and approximately 700 m in the east). Since the groundwater flow direction is generally north to south, the transport domain will extend from a point midway between the waste panels and the northern WIPP boundary to approximately 1000 m beyond the southern

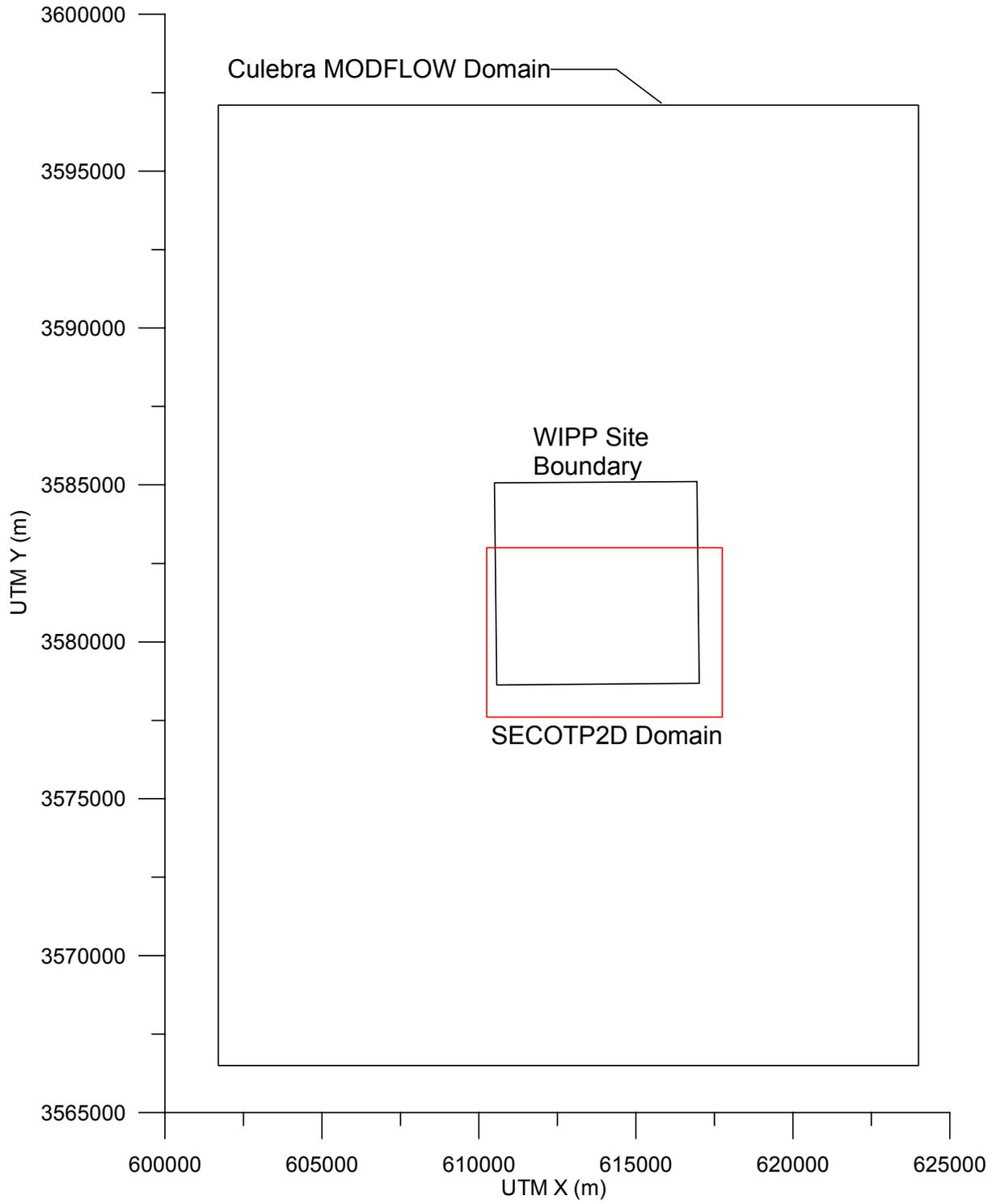


Figure 2. MODFLOW and SECOTP2D domains for the CRA.

WIPP boundary. The transport calculations will use a uniform computational grid composed of 50-m by 50-m cells.

3. TASKS

The work that is covered under this AP is follow-on work to that conducted under AP-088. AP-088 outlines the tasks necessary to generate new T fields for the CRA. Once the T-fields are generated and have been modified for both full- and partial-mining conditions, several additional steps are involved in adapting them for use in the Culebra transport calculations. This analysis plan outlines the tasks necessary to use the new T fields in the Culebra transport calculations. The input from the work performed under AP-088 for the tasks outlined here are 100 unaltered T fields, 100 T fields altered for the full mining scenario, and 100 T fields altered for the partial mining scenario.

3.1 TASK 1: ACCEPTANCE CRITERIA FOR CALIBRATED T FIELDS

The T fields generated under AP-088 represent the best calibrations that can be practicably achieved by PEST subject to the imposed constraints. The primary constraint limiting PEST's ability to achieve a good calibration is the starting base T field itself. The base T fields, generated under Task 2 of AP-088, represent realizations of the true T field based on our knowledge of the geology of the area and inferred values of transmissivity. The calculated T fields are not constrained, however, by the transient response data that are used to calibrate the base T fields, so they cannot be considered "equally probable" when those data are taken into account. In fact, the transient-calibration process reveals that some of the base T fields are such poor representations of the true field that they cannot be well-calibrated at all.

For the CRA calculations, only T fields meeting objective calibration criteria will be used. The acceptance criteria for the T fields will involve comparisons of the modeled and measured steady-state and transient heads, the model calibration objective function, and relationships between these factors and groundwater travel time. The product of this task will be a records package documenting the development and application of the acceptance criteria.

3.2 TASK 2: CONVERSION TO 50-M GRID

The T fields being generated under AP-088 use a uniform grid of 100-m by 100-m cells. The radionuclide transport calculations require a more refined grid with 50-m by 50-m cells. Hence, the MODFLOW domain used for T-field generation will be refined by creating a new grid with 50-m by 50-m cells, and mapping the T values from each of the old 100-m by 100-m cells directly into four 50-m by 50-m cells. The fixed-head boundary conditions for the refined grid will be defined through linear interpolation of the heads assigned for the 100-m grid.

The product of this task will be 300 T fields on a 50-m grid: 100 T fields that have met the acceptance criteria defined under Task 1 that are unaltered for any mining, the same 100 T fields altered for partial mining (outside the controlled area), and the same 100 T fields altered for full mining (both inside and outside the controlled area).

3.3 TASK 3: MODFLOW RUNS TO GENERATE SECOTP2D INPUT

After the AP-088 T fields are migrated to the 50-m grid, a forward steady-state MODFLOW run will be performed for each field to generate a cell-by-cell water-budget file that can be used as input to SECOTP2D. The product of this task will be 300 water-budget files.

3.4 TASK 4: EXTRACTION OF FLOW FIELD VALUES FOR SECOTP2D

Because the physical domain used in the transport calculations will be a subregion of that used for the groundwater flow calculations, the water budget information for the transport subregion will be extracted from the full water budget files calculated by MODFLOW. The product of Task 5 will be 300 extracted water budget files: 100 for unaltered conditions; 100 for partial-mining conditions; and 100 for full-mining conditions.

3.5 TASK 5: SCALING FOR CLIMATE CHANGE

This task involves application of a scaling factor to the groundwater velocity fields from Task 4 to account for climate change, and calculation of radionuclide transport through the Culebra.

Section 6.4.9 of the CCA (DOE, 1996) discusses how potential changes in the future climate might affect groundwater flow in the Culebra, and how the effects of those changes are incorporated in transport modeling. The regional, three-dimensional effects of climate change can be reasonably approximated in performance assessment through direct scaling of specific discharge in the two-dimensional, steady-state groundwater velocity field for the Culebra. Radionuclide transport in the Culebra is then calculated by SECOTP2D using the scaled velocity fields.

Scaling of the two-dimensional velocity field is done using the Climate Index, which is a dimensionless factor by which the specific discharge in each grid block of the MODFLOW domain is multiplied. As summarized in CCA Appendix PAR (Parameter 48), the Climate Index 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. A single value of the Climate Index is chosen in LHS for each sample element and held constant throughout the 10,000-year SECOTP2D simulation. Each realization of disposal system performance thus represents a different approximation of future climate. Those realizations (25%) in which the sampled value is close to its maximum of 2.25 represent the most extreme changes in groundwater flow that may result from climatic change. Sampled values close to the minimum of 1.00 (75%) represent climatic changes that have little effect on groundwater-flow velocities. Because all sampled values of the Climate Index are greater than 1.00, climate change as implemented in the performance assessment can only increase the rate of groundwater flow. The Climate Index is applied to each velocity field by the code PRESECOTP2D.

3.6 TASK 6: RADIONUCLIDE TRANSPORT CALCULATIONS

Radionuclide transport in the Culebra will be calculated using SECOTP2D. SECOTP2D will be run for 600 cases: three replicates of 100 vectors each for both full- and partial-mining conditions. Each replicate applies a different random sampling of the Climate Index to the velocity fields. The output from the SECOTP2D calculations will be used in CCDFGF to calculate the CCDF for releases through the Culebra over 10,000 years. The results of Task 6 will be documented in an analysis package.

The schedule, tasks, and responsible individuals are outlined in Table 2.

Table 2. Tasks and Responsibilities.

Estimated Completion Date	Task(s)	Responsible Individual
June 30, 2003	Acceptance Criteria for Calibrated T Fields	Rick Beauheim
June 30, 2003	Conversion to 50-m Grid	Tom Lowry
June 30, 2003	MODFLOW Runs to Generate SECOTP2D Input	Tom Lowry
July 10, 2003	Extraction of Flow-field values for SECOTP2D	Joe Kanney
July 10, 2003	Application of Climate Index	Joe Kanney
July 31, 2003	Calculation of Radionuclide Transport in the Culebra	Joe Kanney

4. PARAMETERS USED IN CULEBRA TRANSPORT CALCULATIONS

The Culebra flow calculations are run to create input files for the Culebra transport calculations. The Culebra transport calculations also use parameters from the Performance Assessment Parameter Database (PAPDB). A list of the parameters used in the Culebra transport calculations is given in Table 3. Parameters that are listed as sampled parameters will be sampled using LHS. The parameters used in the Culebra calculations are the same as those used in the CCA with the exception of the matrix distribution coefficients noted below.

Table 3. Parameters Used In SECOTP2D.

Material	Property	Description	Value
CULEBRA	APOROS	Advective porosity	Sampled
CULEBRA	DPOROS	Diffusive porosity	Sampled
CULEBRA	DISP_L	Longitudinal dispersivity (m)	0.0
CULEBRA	DISPT_L	Transverse dispersivity (m)	0.0
CULEBRA	FTORT	Fracture tortuosity	1.0
CULEBRA	DTORT	Diffusive tortuosity	0.11
CULEBRA	HMBLKL	Half-matrix block length (m)	Sampled
CULEBRA	SKIN_RES	Skin resistance	0.0
CULEBRA	DNSGRAIN	Material grain density (kg/m ³)	2820
GLOBAL	OXSTAT	Oxidation state index	Sampled
GLOBAL	CLIMTIDX	Climate index	Sampled
REFCON	YRSEC	Seconds per year (s/yr)	3.155693E+07
AM241	ATWEIGHT	Atomic weight (kg/mole)	2.4105700E-01
AM241	HALFLIFE	Half-life (s)	1.3640000E+10
PU239	ATWEIGHT	Atomic weight of ²³⁹ Pu (kg/mole)	2.3905200E-01
PU239	HALFLIFE	Half-life of ²³⁹ Pu (s)	7.5940000E+11
TH230	ATWEIGHT	Atomic weight of ²³⁰ Th (kg/mole)	2.3003300E-01
TH230	HALFLIFE	Half-life of ²³⁰ Th (s)	2.4300000E+12
U234	ATWEIGHT	Atomic weight of ²³⁴ U (kg/mole)	2.3404100E-01
U234	HALFLIFE	Half-life of ²³⁴ U (s)	7.7160000E+12
AM+3	MKD_AM	Matrix retardation coefficient	Sampled
AM+3	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	3E-10
PU+3	MKD_PU	Matrix retardation coefficient	Sampled
PU+3	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	3E-10
PU+4	MKD_PU	Matrix retardation coefficient	Sampled
PU+4	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	1.53E-10
TH+4	MKD_TH	Matrix retardation coefficient	Sampled
TH+4	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	1.53E-10
U+4	MKD_U	Matrix retardation coefficient	Sampled
U+4	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	1.53E-10
U+6	MKD_U	Matrix retardation coefficient	Sampled
U+6	MD0	Molecular diffusion coefficient in pure liquid (m ² /s)	4.26E-10

The matrix distribution coefficients (K_{ds}) for the actinides between the aqueous and solid phases are parameters of considerable concern. The parameters for the matrix distribution coefficients are defined in Table 4. The K_{ds} are used in the SECOTP2D code (see Hansen and Leigh, 2003).

Table 4. Definition of the Matrix Distribution Parameters.

Parameter Identifier ^(a)	
AM+3/MKD_AM	K _d for Am in the +III oxidation state
NP+4/MKD_NP	K _d for Np in the +IV oxidation state
NP+5/MKD_NP	K _d for Np in the +V oxidation state
PU+3/MKD_PU	K _d for Pu in the +III oxidation state
PU+4/MKD_PU	K _d for Pu in the +IV oxidation state
TH+4/MKD_TH	K _d for Th in the +IV oxidation state
U+4/MKD_U	K _d for U in the +IV oxidation state
U+6/MKD_U	K _d for U in the +VI oxidation state

^(a)The material name is listed first followed by the property name

The matrix distribution coefficients for the actinides in the Culebra were developed as a result of experiments at LANL and SNL (Brush, 1996). The K_d values used in the CCA and PAVT are summarized in Table 5. A uniform distribution over the specified range was assumed for all matrix distribution coefficients.

Table 5. Matrix Distribution Coefficient Ranges and Distributions in the CCA and PAVT.

Parameter Description	Parameter Identifier ^(a)	CCA Value	PAVT Value
Matrix Distribution Coefficient for Am(III)	AM+3/MKD_AM	0.02-0.5 m ³ /kg Uniform	0.02-0.5 m ³ /kg Log Uniform
Matrix Distribution Coefficient for Np(IV)	NP+4/MKD_NP	0.9-20 m ³ /kg Uniform	0.9-20 m ³ /kg Log Uniform
Matrix Distribution Coefficient for Np(V)	NP+5/MKD_NP	0.001-0.2 m ³ /kg Uniform	0.001 - 0.2 m ³ /kg Log Uniform
Matrix Distribution Coefficient for Pu(III)	PU+3/MKD_PU	0.02-0.5 m ³ /kg Uniform	0.02-0.5 m ³ /kg Log Uniform
Matrix Distribution Coefficient for Pu(IV)	PU+4/MKD_PU	0.9-20 m ³ /kg Uniform	0.9-20 m ³ /kg Log Uniform
Matrix Distribution Coefficient for Th(IV)	TH+4/MKD_TH	0.9-20 m ³ /kg Uniform	0.9-20 m ³ /kg Log Uniform
Matrix Distribution Coefficient for U(IV)	U+4/MKD_U	0.9-20 m ³ /kg Uniform	0.9-20 m ³ /kg Log Uniform
Matrix Distribution Coefficient for U(VI)	U+6/MKD_U	0.00003-0.03 m ³ /kg Uniform	0.00003-0.03 m ³ /kg Log Uniform

^(a)The material name is listed first followed by the property name.

Subsequent to the PAVT, two errors were found in the procedures used to calculate the matrix K_{ds} after they were submitted for the CCA calculations. First, a brine density of 1.00 g/mL was used rather than the measured brine density, and, second, incorrect values for the mass of dolomite were incorporated (Brush and Storz, 1996). The erroneous use of these values led to incorrectly calculated distribution coefficients. However, the influence of the changes in these values on the distribution coefficients was calculated and reported as minimal (Brush and Storz, 1996). These errors were corrected in the values calculated by Brush and Storz (1996).

For some isotopes, Brush and Storz calculated K_{ds} for both deep (Castile or Salado) and Culebra brines. To remain conservative and consistent with the CCA, the CRA will use the range of K_d values for the brine that has the smaller mean value. Probability distributions for all of the matrix distribution coefficients are log uniform distributions, based upon EPA directives for the PAVT. The matrix distribution coefficients for the CRA are listed in Table 6.

Table 6. Matrix Distribution Coefficient Ranges and Distributions in the CRA.

Parameter Description	Parameter Identifier ^(a)	RPB Value	Probability Distribution
Matrix Distribution Coefficient for Am(III)	AM+3/MKD_AM	0.02-0.4 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for Np(IV)	NP+4/MKD_NP	0.7-10 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for Np(V)	NP+5/MKD_NP	0.001-0.2 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for Pu(III)	PU+3/MKD_PU	0.02-0.4 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for Pu(IV)	PU+4/MKD_PU	0.7-10 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for Th(IV)	TH+4/MKD_TH	0.7-10 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for U(IV)	U+4/MKD_U	0.7-10 m ³ /kg	Log Uniform
Matrix Distribution Coefficient for U(VI)	U+6/MKD_U	0.00003-0.02 m ³ /kg	Log Uniform

^(a)Values include correction for brine density and mass of dolomite (Brush and Storz, 1996).

5. SOFTWARE LIST

The major codes to be used for the CRA Culebra calculations are listed in Table 7. All code calculations except those using MODFLOW-2000 and PEST will be performed on qualified ES-40, ES-45 or 8400 Alpha computers running OpenVMS 7.3-1. MODFLOW-2000 and PEST will be run on PCs using i686 CPUs running Red Hat linux 7.2.

Table 7. Codes to be Used in the CRA Culebra Flow and Transport Analysis.

Code	Version
ALGEBRACDB	2.35
GENMESH	6.08
LHS	2.41
MATSET	9.10
MODFLOW-2000	1.60
PEST	5.51
PRELHS	2.30
PRESECOTP2D	1.22
POSTLHS	4.07
SECOTP2D	1.41

6. SPECIAL CONSIDERATIONS

None.

7. APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow NP 9-2. The database will be managed in accordance with relevant technical procedure.

Computer Codes: New or revised computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. All other codes unchanged since the PAVT are qualified under multi-use provisions of NP 19-1. Codes other than MODFLOW-2000 and PEST will be run on fully qualified ES-40 and/or ES-45 DEC ALPHA computers running Open VMS Version 7.3-1. MODFLOW-2000 and PEST will be run on PCs using i686 CPUs running Red Hat linux 7.2

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

8. REFERENCES

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