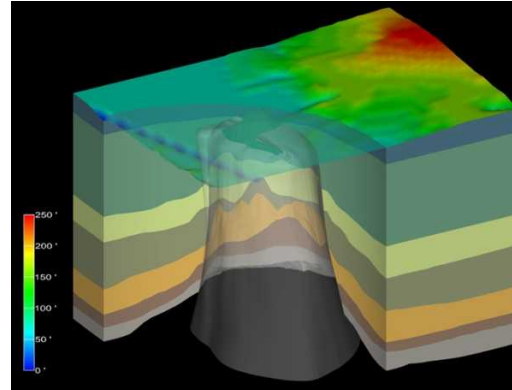


Exceptional service in the national interest

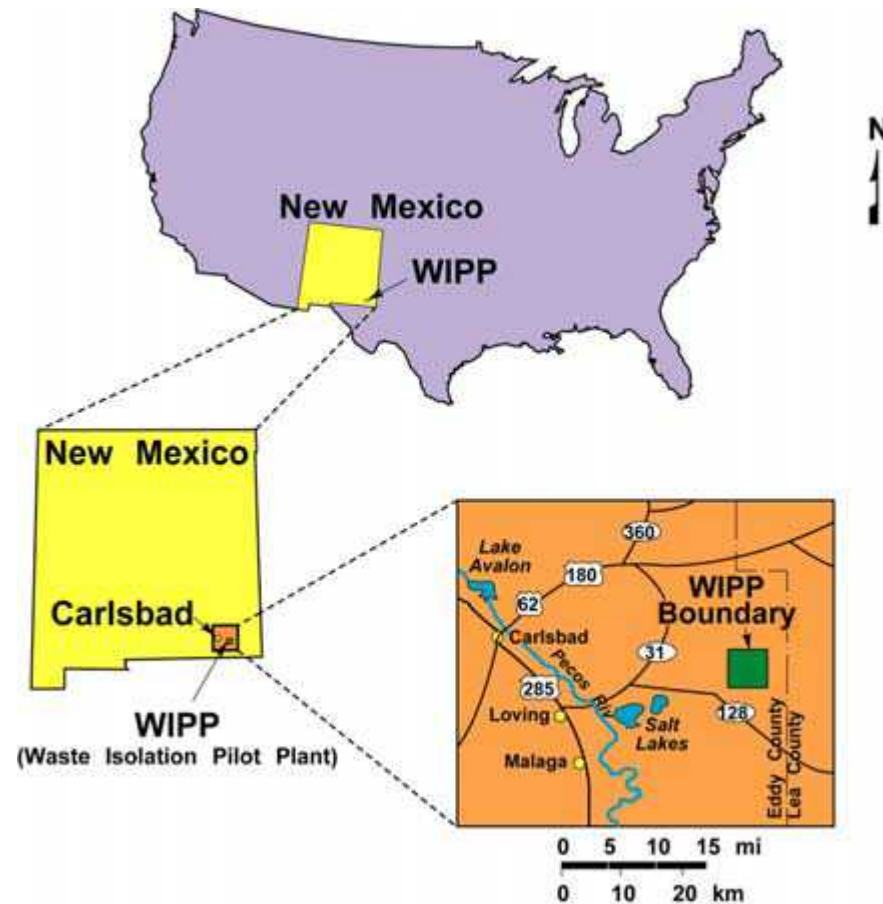


Example Applications of Geostatistics in Repository Safety Assessments and Summary of Key Conclusions Regarding Safety Assessment and Site Characterization

IAEA Training Course – July 1-5, 2013

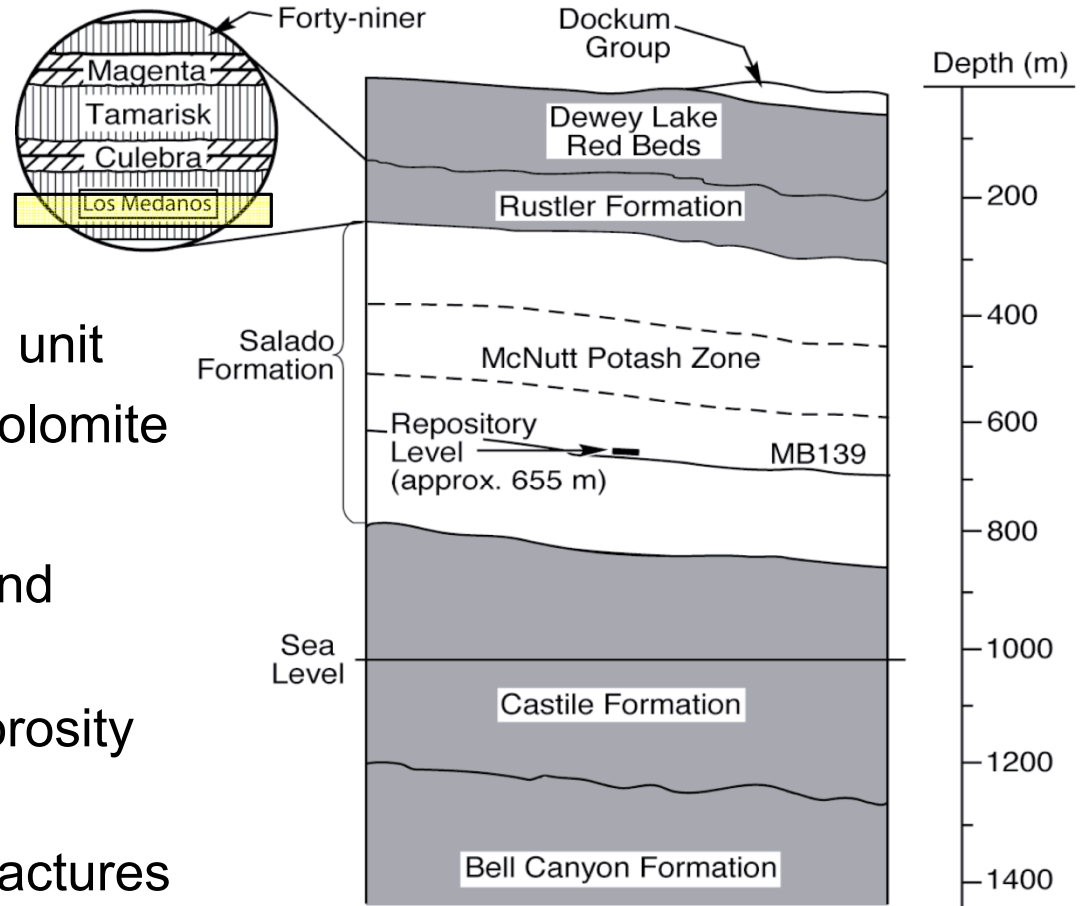
Robert J. MacKinnon

Waste Isolation Pilot Plant (WIPP)



1404-2

Rustler Formation in WIPP Vicinity

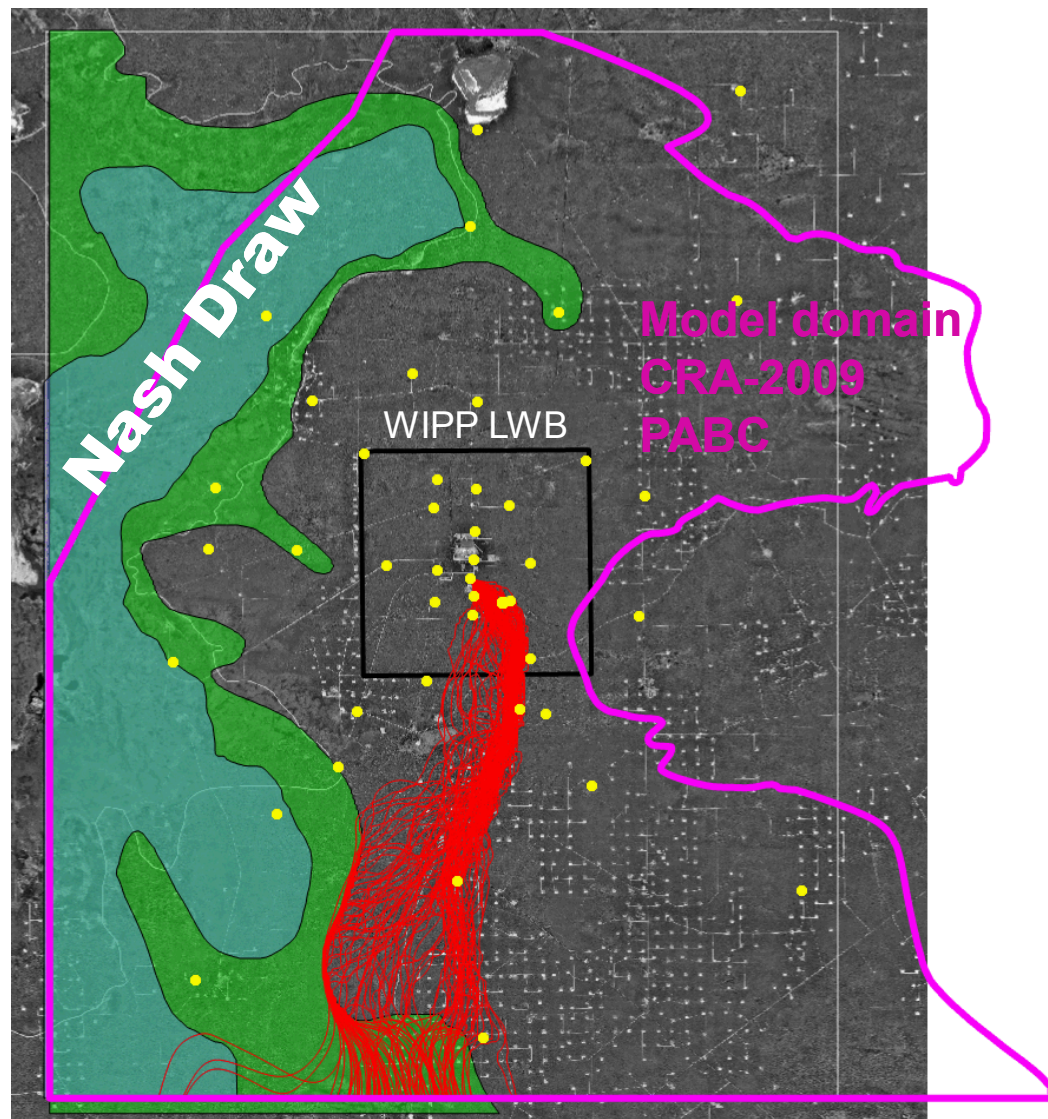


Culebra Formation

- Most transmissive saturated unit
- 7.75 meter thick fractured Dolomite
- 4 meter thick transport zone
- Multiple scales of porosity and permeability
- Tracer tests indicate dual porosity behavior
 - Advective transport in fractures
 - Diffusive transport in rock matrix

Culebra Flow Modeling Domain

- Culebra at WIPP
 - confined
 - no leakage
 - no recharge
- Nash Draw
 - Karst / sinkholes
 - some recharge
 - unconfined
- Culebra flow is N-S



2-D Transient Groundwater Flow Equations

$$S \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} \left(T \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial \phi}{\partial y} \right) + Q(x, y, t)$$

$$\phi = z + \frac{p}{\gamma}$$

$$T = Kb$$

where:

$\phi \equiv$ potentiometric head [L]

$z \equiv$ elevation [L]

$p \equiv$ pressure [ML⁻¹T⁻²]

$\gamma \equiv$ specific weight of water [ML²T⁻²]

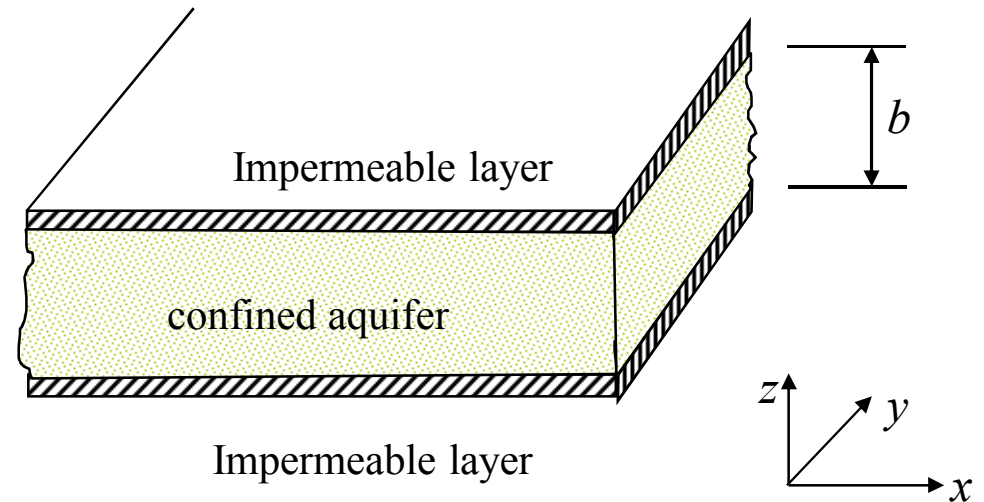
$S \equiv$ aquifer storativity [-]

$T \equiv$ aquifer transmissivity [L²T⁻¹]

$K \equiv$ hydraulic conductivity [LT⁻¹]

$b \equiv$ aquifer thickness [L]

$Q \equiv$ source/sink per unit area [LT⁻¹]



Overview of T-field Development

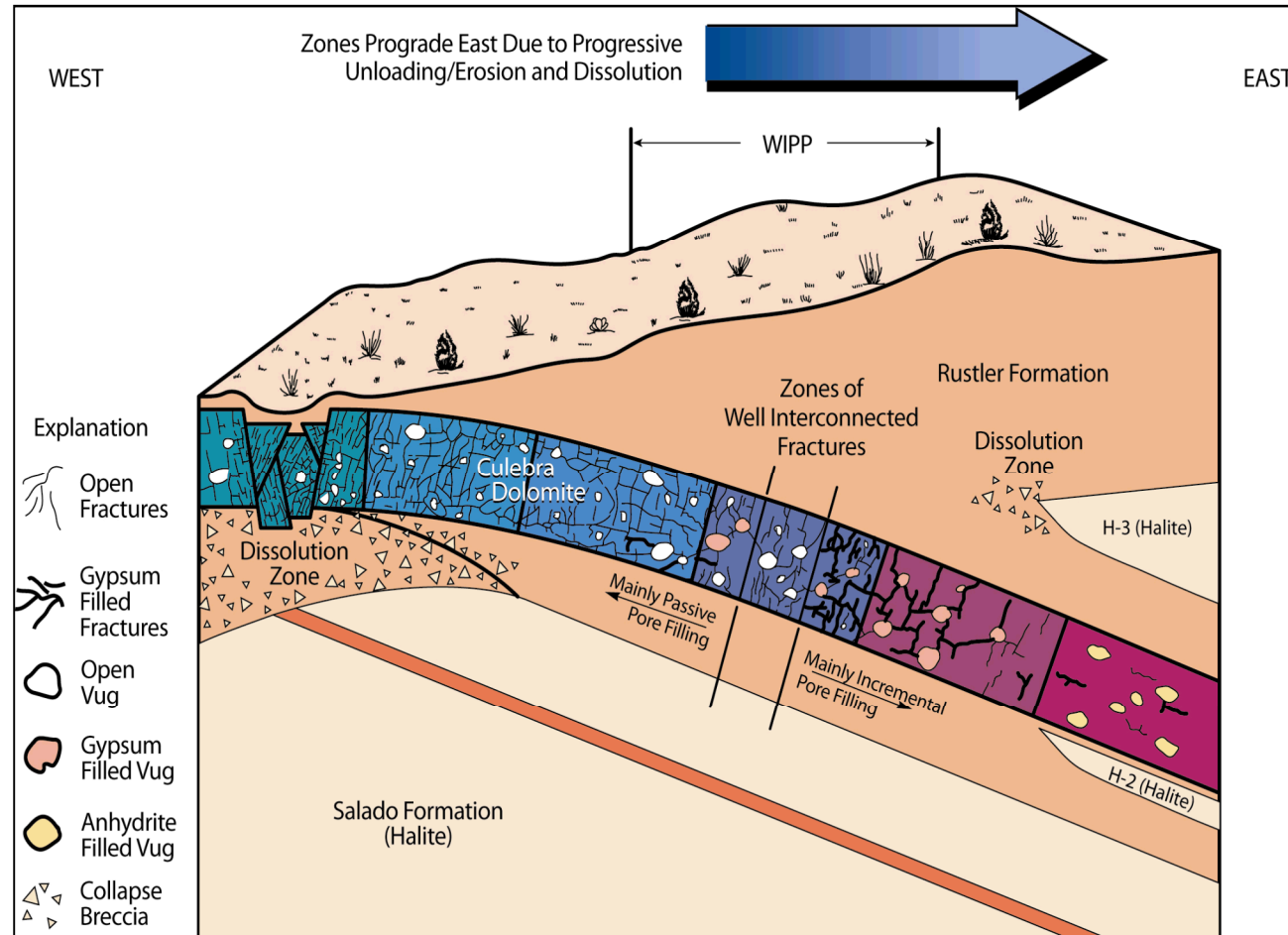
- Starting point in the T-field development process was to assemble and update information on geologic factors potentially affecting Culebra T
 - dissolution of the upper Salado Formation located below the Culebra
 - presence of gypsum cements
 - thickness of overburden above the Culebra
 - spatial distribution of halite in the Rustler Formation both above and below the Culebra
- Geologic information is available from hundreds of oil and gas wells and potash exploration holes in the vicinity of the WIPP site, while estimates of Culebra T are available from only 64 well locations.

Overview of T-field Development

- A two-part geologically based approach was used to generate base Culebra T-fields.
 1. A conceptual model for geologic controls (i.e., soft data) on Culebra *T* was developed, and the hypothesized geologic controls were regressed against Culebra *T* estimates at monitoring wells to determine linear regression model (coefficients)
 2. The regression model was then combined with the maps of geologic factors to create stochastically varying base Culebra T-fields

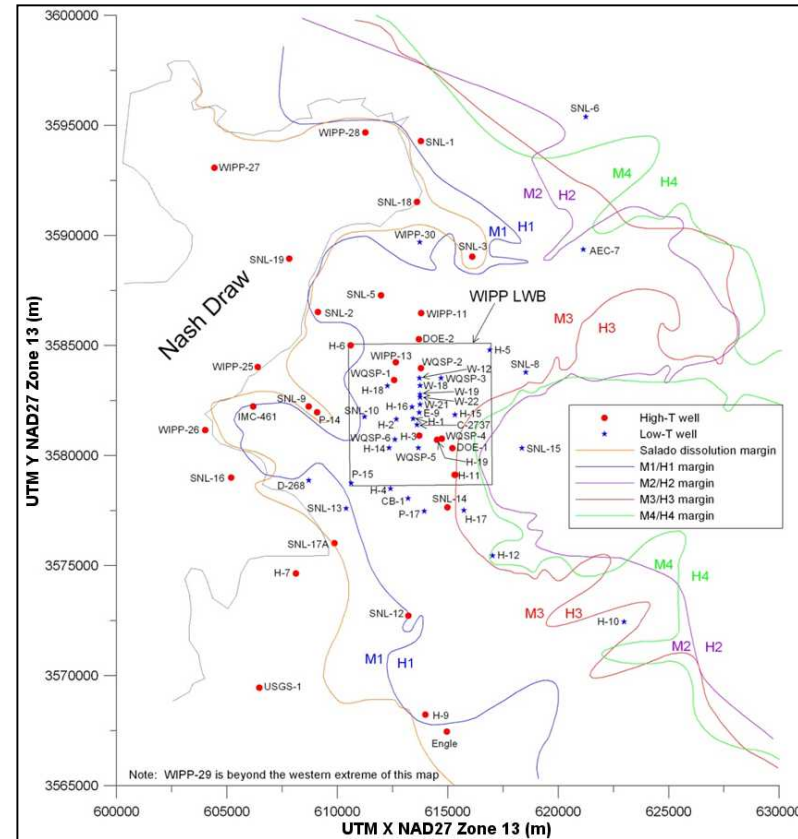
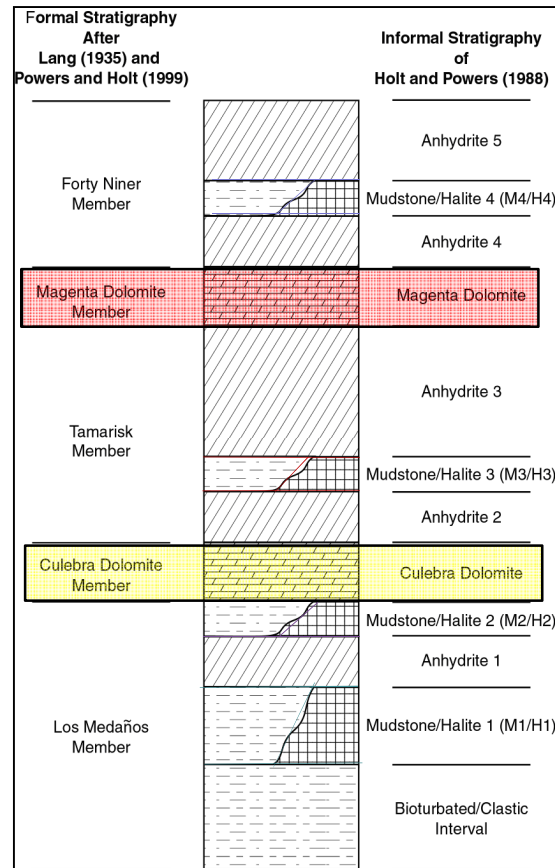
Geologic Conceptual Model

- Increase in permeability (west) due to dissolution of Salado
- Decrease in permeability (east) due to interbedded evaporites and overburden thickness
- WIPP site is located between these two zones



Geologic Conceptual Model

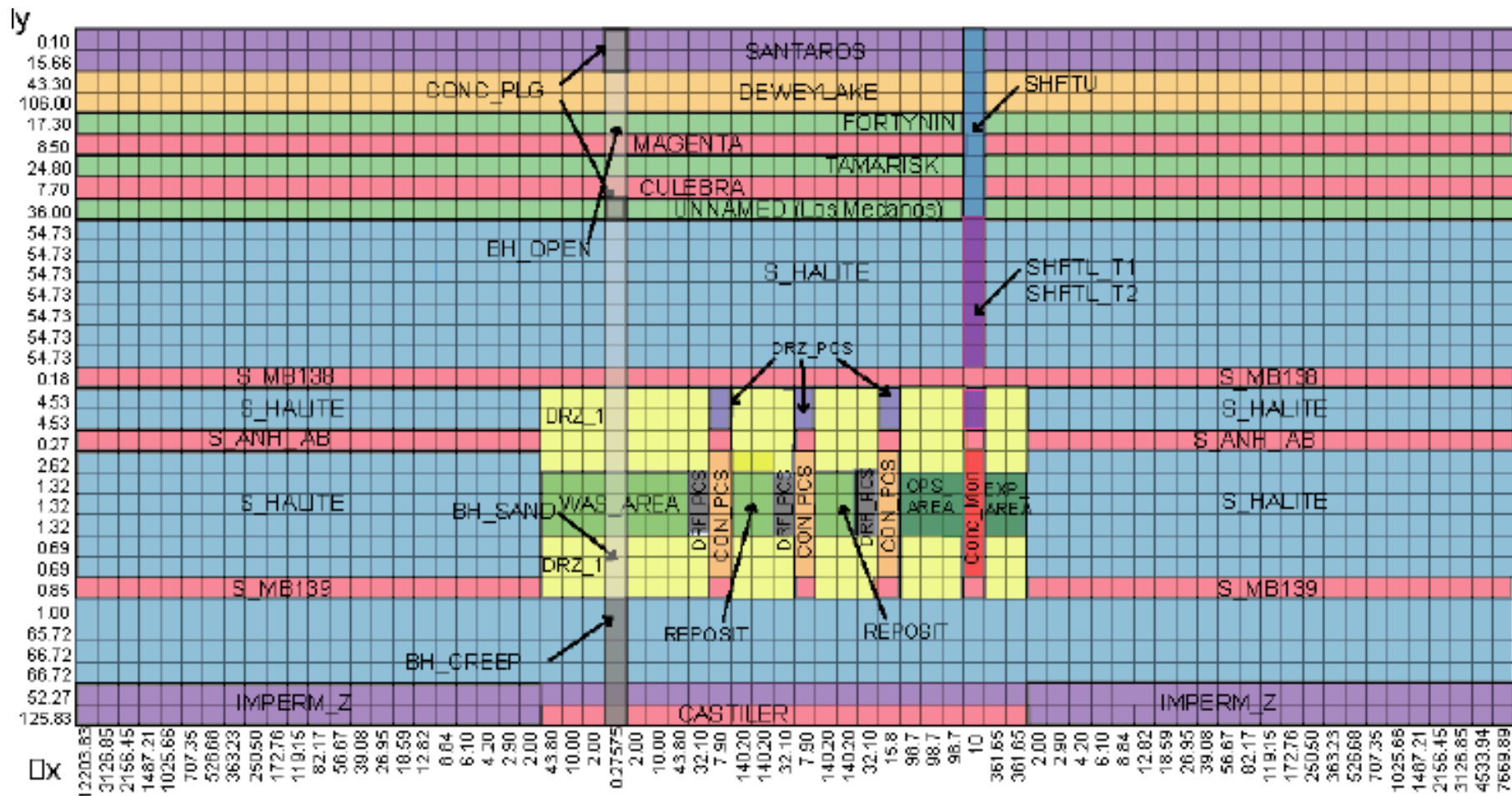
- Lateral changes in Rustler geology are facies changes, not evaporite dissolution (Holt & Powers, 1988)
- Mudstone / Halite boundaries defined with >100 WIPP boreholes + logs from thousands of oil & potash boreholes (Powers, 2007)



Culebra Conceptual Model

- The Culebra Member of the Rustler Formation is considered as a potential long-term release pathway in WIPP PA, because it is the most permeable laterally continuous geologic unit above the WIPP repository level.
- Potential future human intrusion into the repository might connect the repository with the Culebra, which would then transport radionuclides to the accessible environment under natural flow conditions.
- Groundwater flow in the Culebra is generally from north to south at the WIPP site
- The accessible environment is defined to be where the WIPP Land Withdrawal Boundary (LWB) intersects the Culebra in the subsurface.

WIPP BRAGFLO Cross-Section



Spatial Variability in Transmissivity

- The spatial variability in transmissivity observed in the Culebra is incorporated by assigning different transmissivity values to every computational cell in the model (100-m square cells – 284Wx307H).
- Because there is uncertainty in the estimated value of Culebra transmissivity in areas where measurements have not been made, a large set of transmissivity fields is developed.
- Each transmissivity field is a statistical representation of the natural variation in transmissivity that honors measured data according to certain criteria.
- For a set of transmissivity fields generated with identical constraints, each field is equally likely to represent actual conditions.
- Monte Carlo simulations using a large number of equally-likely transmissivity fields is a statistically sound method of characterizing the uncertainty associated with transmissivity in the Culebra.

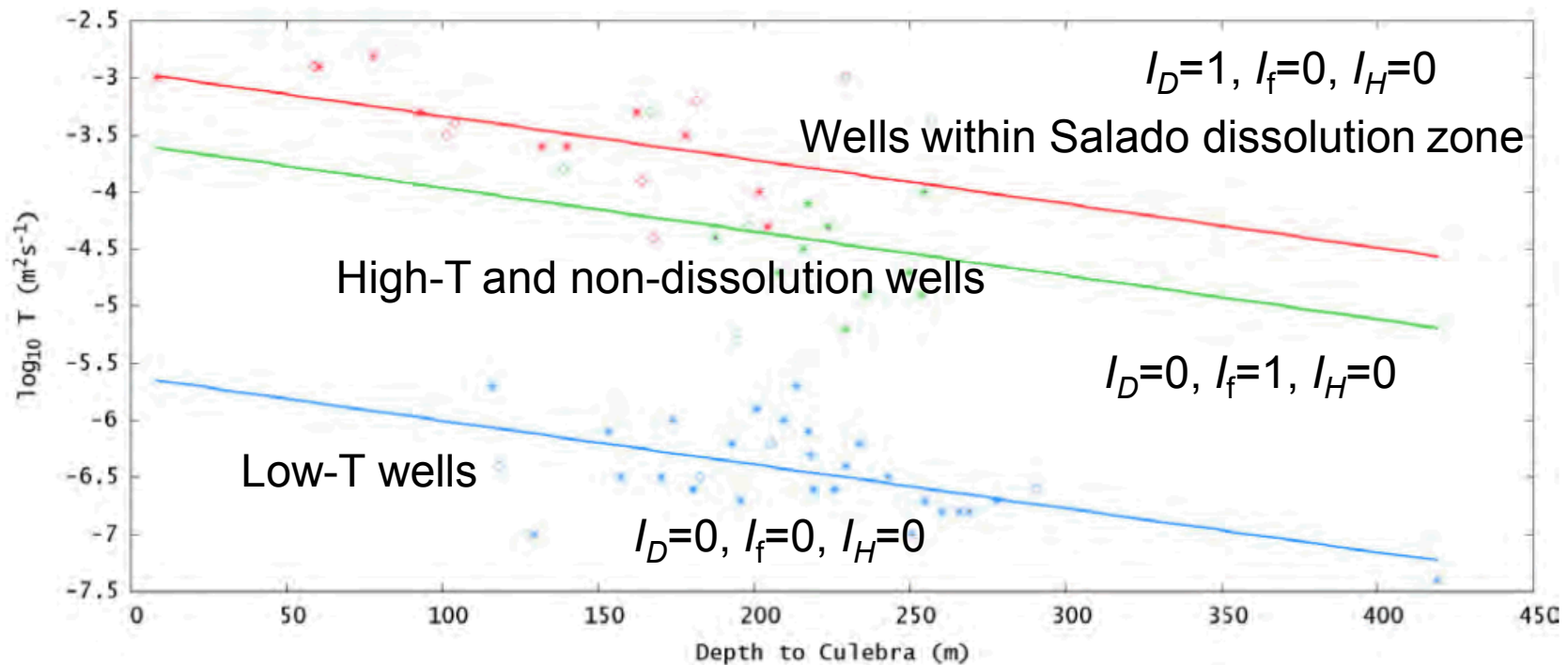
Conceptual Model Refinement

- Hypothesized Culebra T spatial distribution is a function of several geologic factors some of which can be determined at a location using mapped geologic data, including:
 - Dissolution of the upper Salado Formation below the Culebra
 - Presence of gypsum cements in fractures and vuggy porosity
 - Occurrence of halite in Rustler units above or below the Culebra
 - Culebra overburden thickness
 - Fracture interconnection
- Presence of gypsum cements in the Culebra, occurrence of Rustler halite, and Culebra overburden thickness instead varies slowly in space; these properties can be meaningfully mapped at the scale of the groundwater flow model
- *Fracture interconnection is treated as a stochastic process*

Transmissivity Regression Model

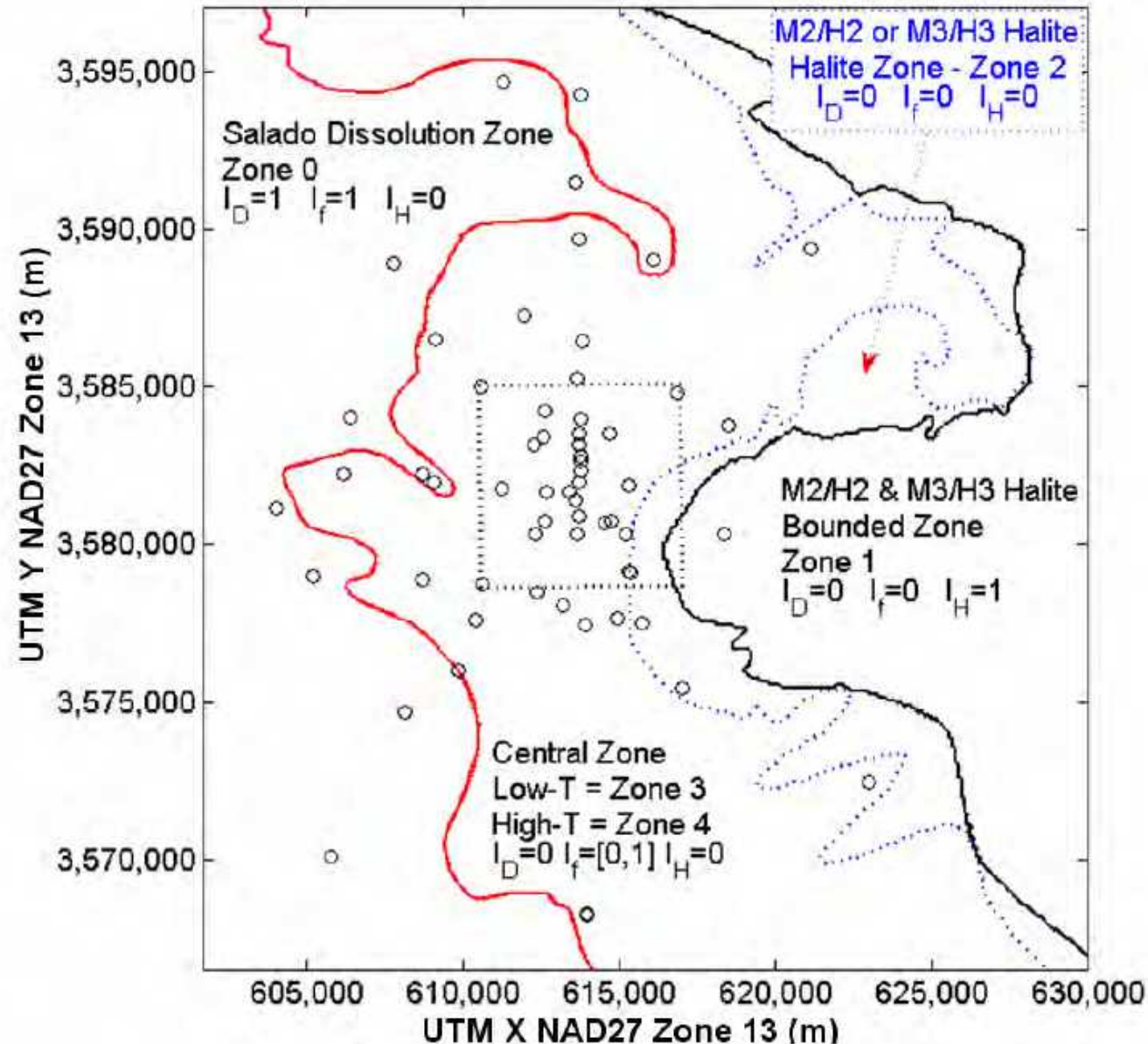
$$Y(x, y) = \beta_1 + \beta_2 d(x, y) + \beta_3 I_f(x, y) + \beta_4 I_D(x, y) + \beta_5 I_H(x, y) + \varepsilon$$

β_1	β_2	β_3	β_4	β_5
-5.69805	-3.48357×10^{-3}	2.06581	0.68589	-4.75095



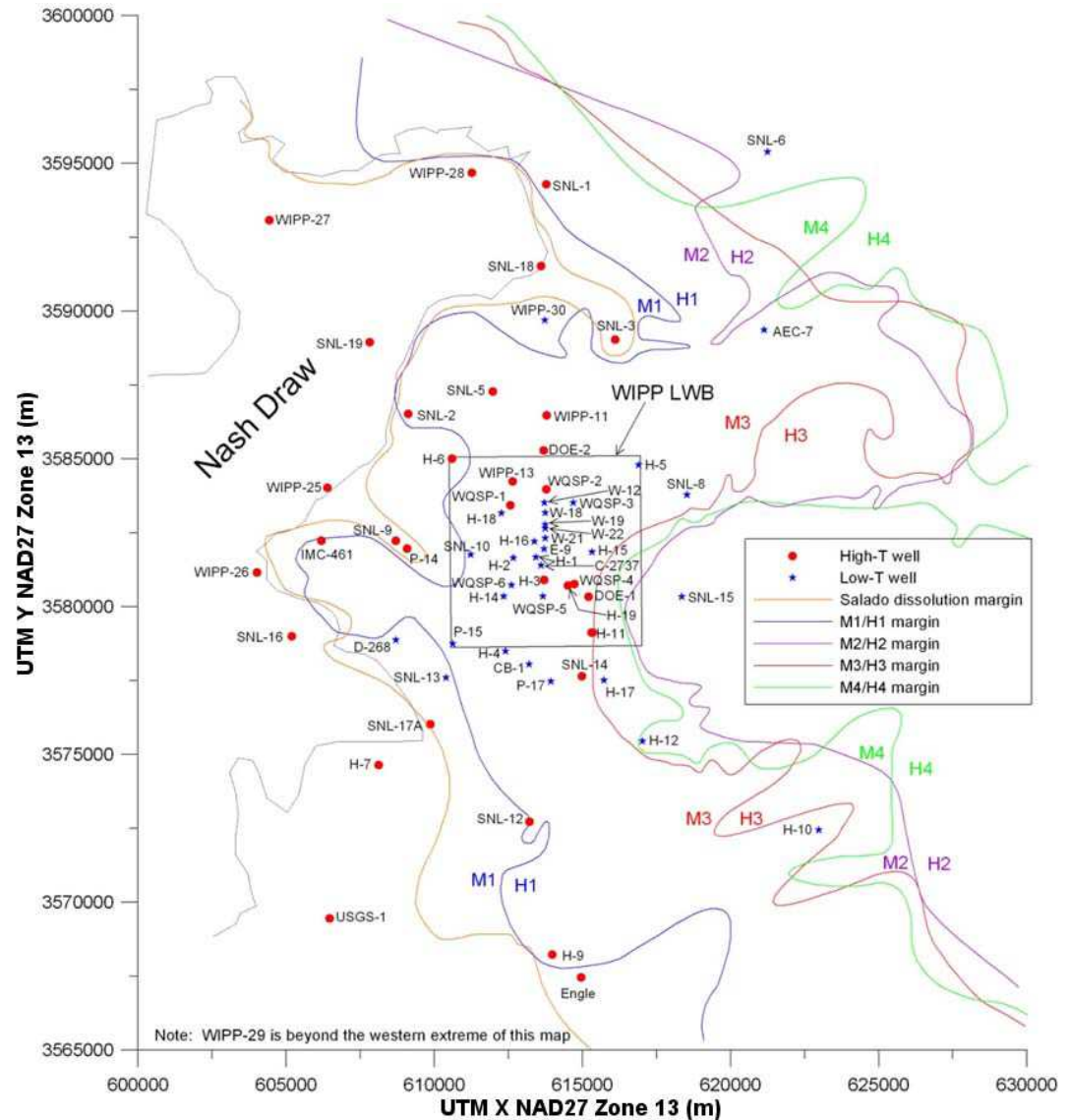
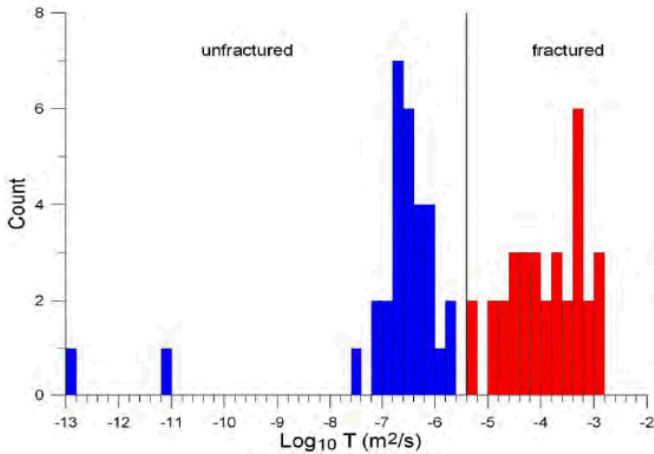
Conceptual model zones with indicator values and zone numbers

Zones 3 and 4 are distributed randomly between the Salado dissolution margin and westernmost of M2/H3 or M3/H3 Rustler halite margins



Histogram of \log_{10} Culebra transmissivity (T) estimates at WIPP wells from single-well tests

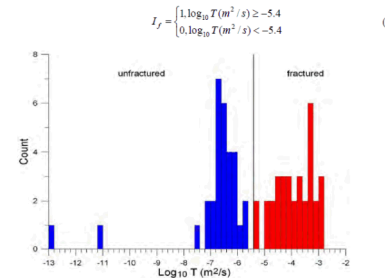
$$I_f = \begin{cases} 1, & \log_{10} T(m^2/s) \geq -5.4 \\ 0, & \log_{10} T(m^2/s) < -5.4 \end{cases}$$



Indicator Variography

- Geostatistical indicator simulations done as part of the base T-field development are only utilized in the central section of the model domain, between the Salado dissolution area to the west and the low-T halite-sandwiched region to the east
- Only wells in this middle section are used for construction of the indicator variogram; a total of 46 wells provide information regarding $\log_{10} T$
- Indicator value is determined by comparing each $\log_{10} T$ value to a threshold $\log_{10} T$ value, $T_t = -5.4$

$$I(x, y) = \begin{cases} 1 & \text{if } \log_{10} T < T_t \\ 0 & \text{if } \log_{10} T \geq T_t \end{cases}$$

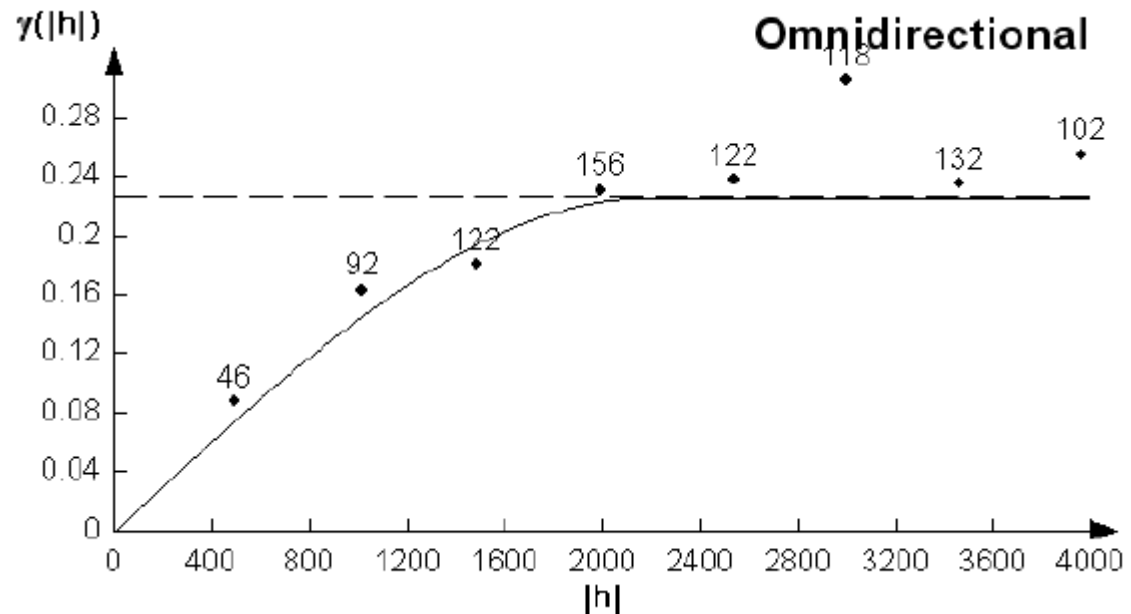


where $I(x, y)$ denotes the unit-less indicator value at well location (x, y)

Indicator Variography

- The experimental indicator variogram was fit with a spherical variogram model
- The proportion of low-T values in the data set is 0.652
- The variance of an indicator value is $(1 - p)p$, where p is the proportion of high or low values; the variance is 0.227 and is used directly as the sill in the variogram modeling

Parameter	Value
Model Type	Spherical
Nugget	0.0
Sill	0.227
Range	2195 m



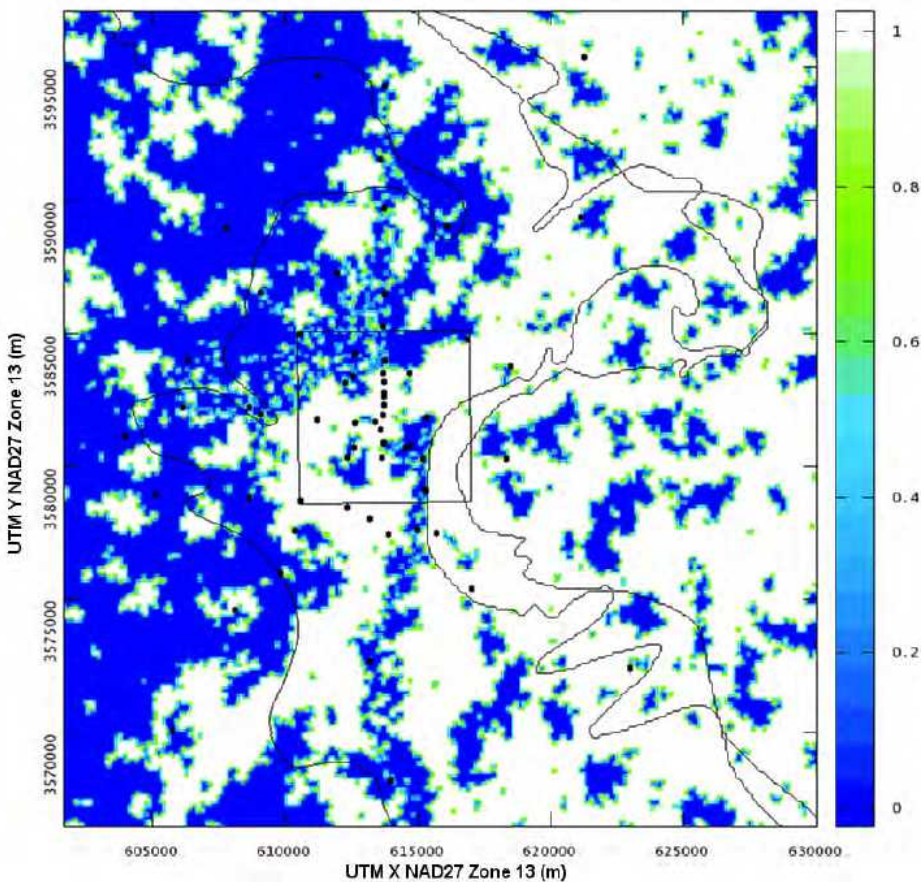
Experimental variogram (dots) and spherical model (line) for indicator values; x-axis is lag distance [meters], y-axis is the unitless indicator; numbers by dots indicate the number of pairs represented at each lag

Partial listing of coordinates, Culebra depth, and $\log_{10} T$ estimates from single-well tests used in regression model

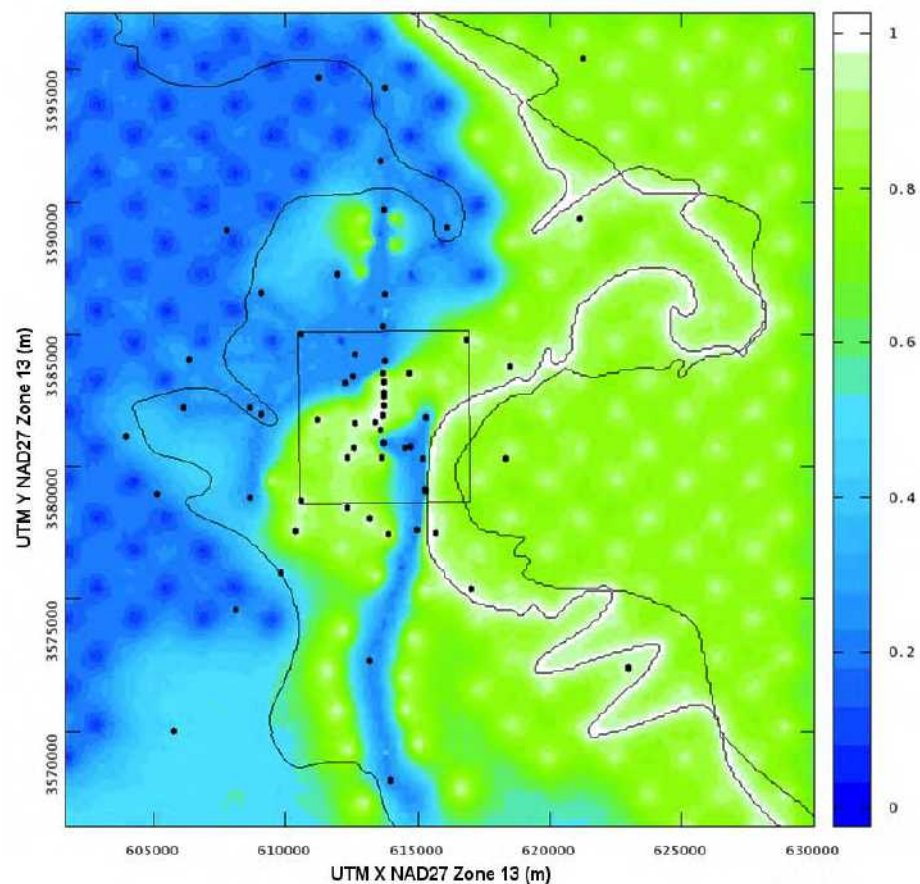
Well	UTM XNAD27, Zone 13 (m)	UTM YNAD27, Zone 13 (m)	depth to Culebra (m)	$\log_{10} T$ (m^2/s)
H-10b	622975	3572473	419.25	-7.4
P-15	610624	3578747	129.24	-7.0
WIPP-12	613710	3583524	250.7	-7.0
AEC-7	621126	3589381	269.14	-6.8
H-15	615315	3581859	265.79	-6.8
WQSP-3	614686	3583518	260.38	-6.8
H-12	617023	3575452	254.97	-6.7
H-5c	616903	3584802	277.82	-6.7
WIPP-30	613721	3589701	195.69	-6.7
H-17	615718	3577513	219.03	-6.6
SNL-8	618523	3583783	291.5	-6.6
WIPP-21	613743	3582319	225.85	-6.6
WQSP-6	612605	3580736	180.31	-6.6
CB-1	613191	3578049	157.27	-6.5
H-14	612341	3580354	170.23	-6.5
SNL-10	611217	3581777	182.58	-6.5
WIPP-18	613735	3583179	243.08	-6.5
SNL-13	610394	3577600	118.26	-6.4
WIPP-22	613739	3582653	229.51	-6.4
ERDA-9	613696	3581958	218.08	-6.3
C-2737	613597	3581401	205.74	-6.2
H-2c	612666	3581668	192.94	-6.2
WIPP-19	613739	3582782	233.93	-6.2

Stochastic Indicator Fields

1 indicates low T and 0 indicates high T



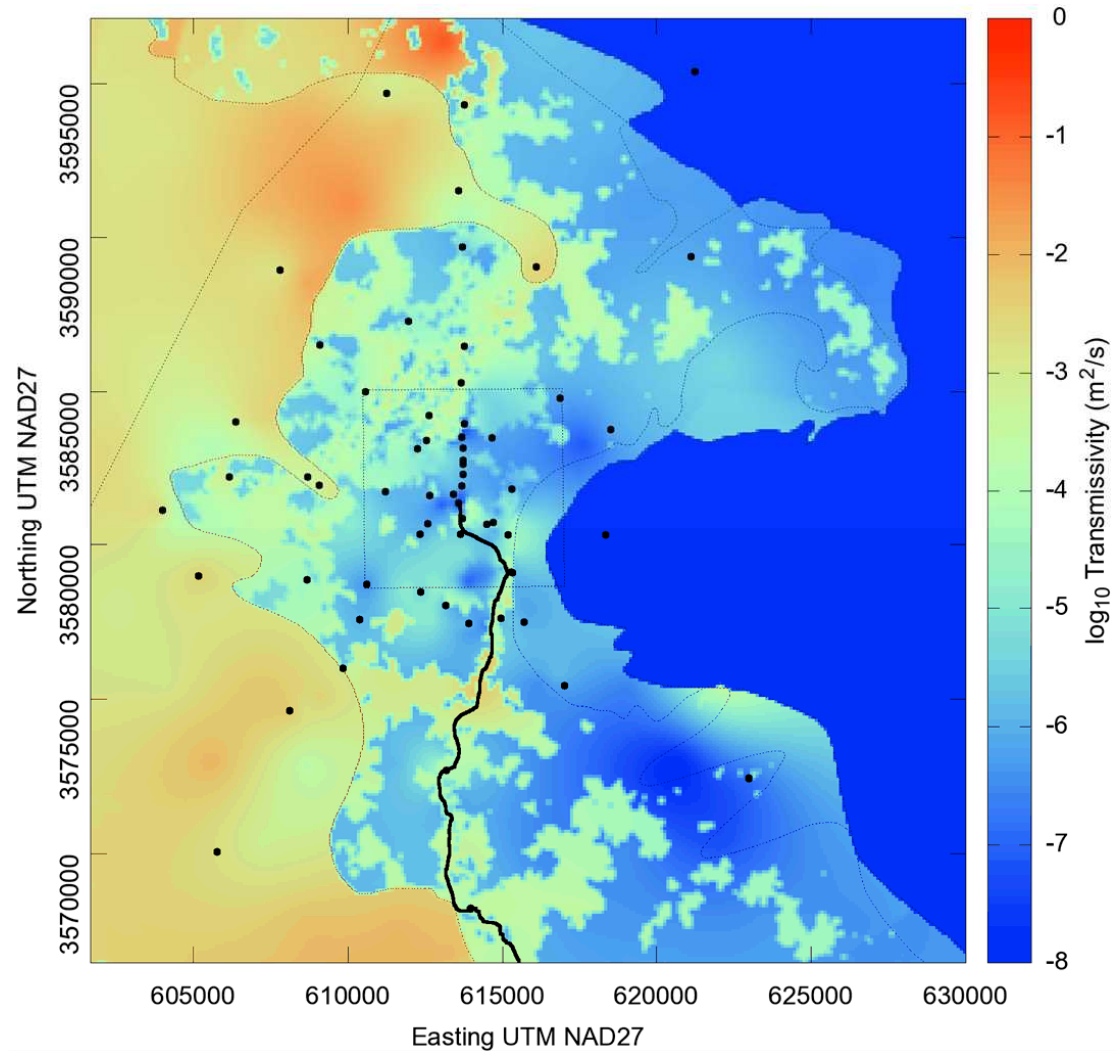
Single Realization



Average indicator values across all 1000 base realizations

Example Culebra T Field

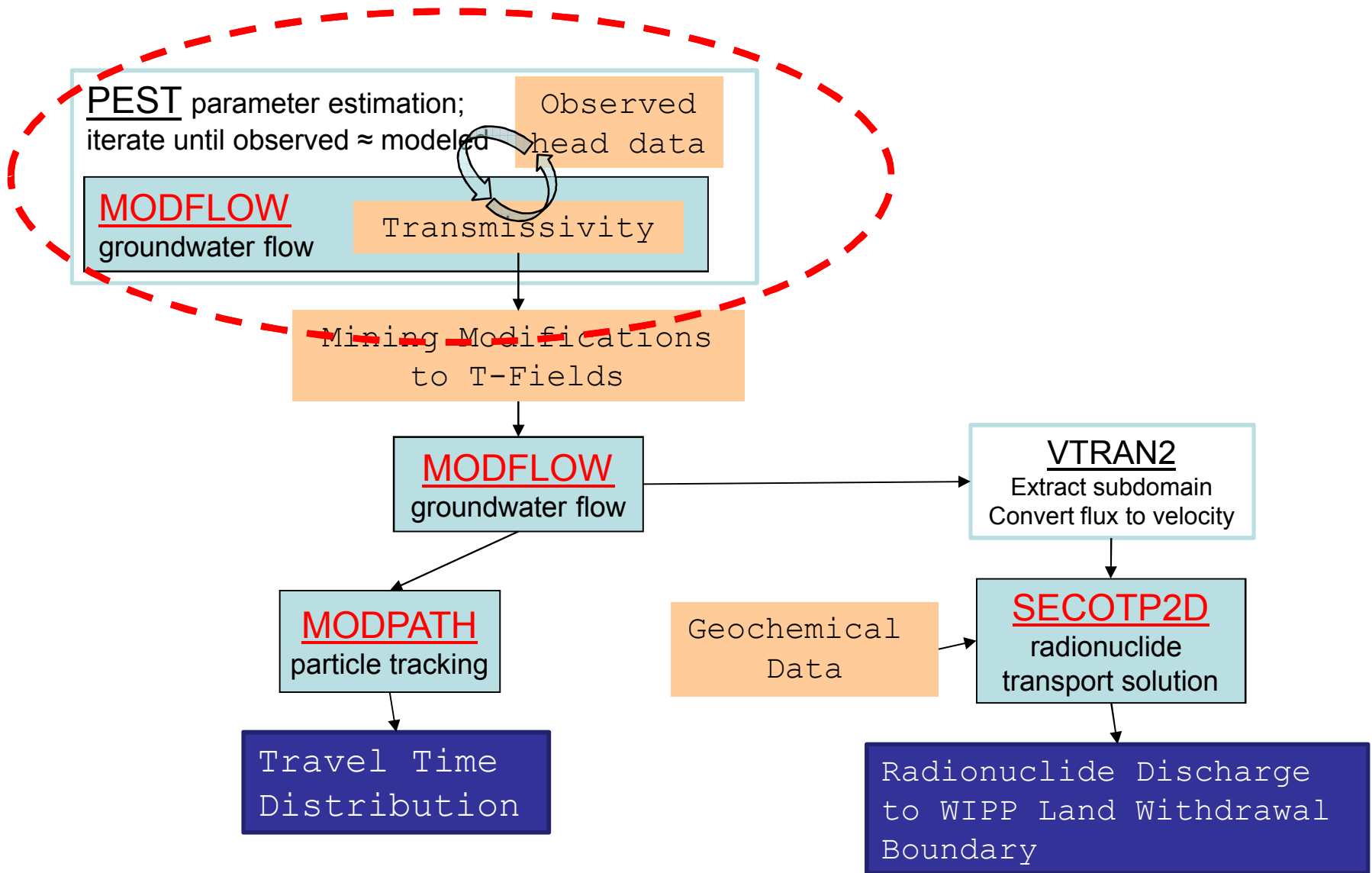
Example Culebra T field used in flow and particle tracking model, with illustrative particle track from the center of the WIPP to the edge of the domain. Black dots are observation well locations.



Subsequent Steps in Numerical Implementation

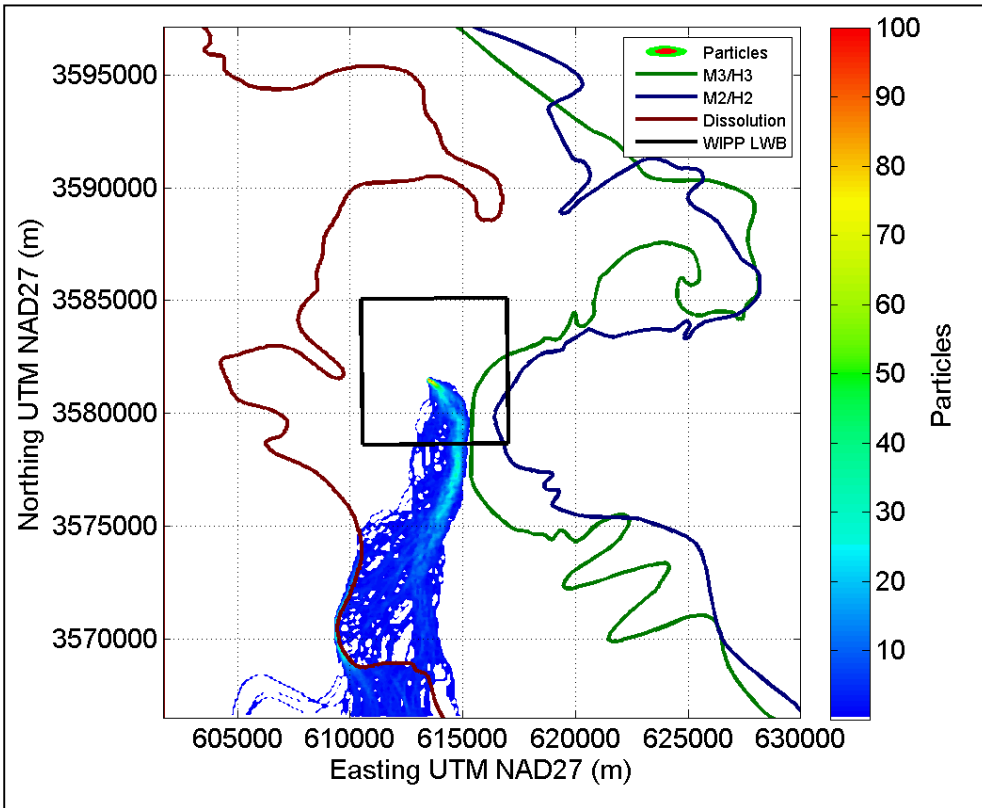
1. T-Field calibration
2. Mining modifications
3. Flow and particle tracking calculations
4. Radionuclide transport

Transmissivity Field Calibration

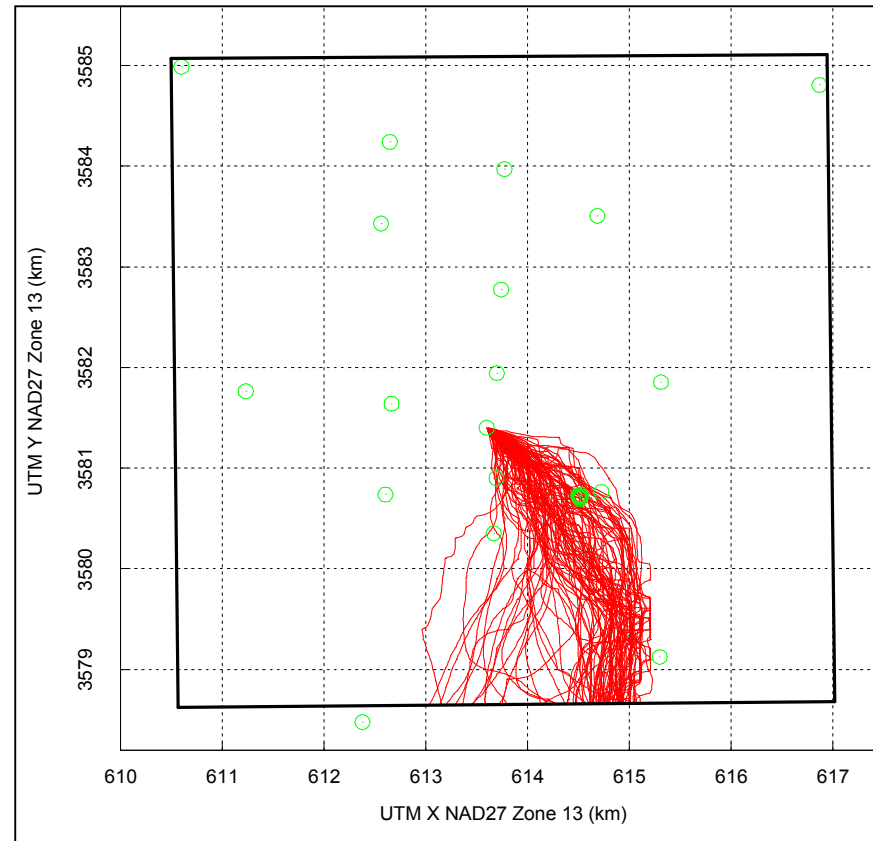


Particle Tracks

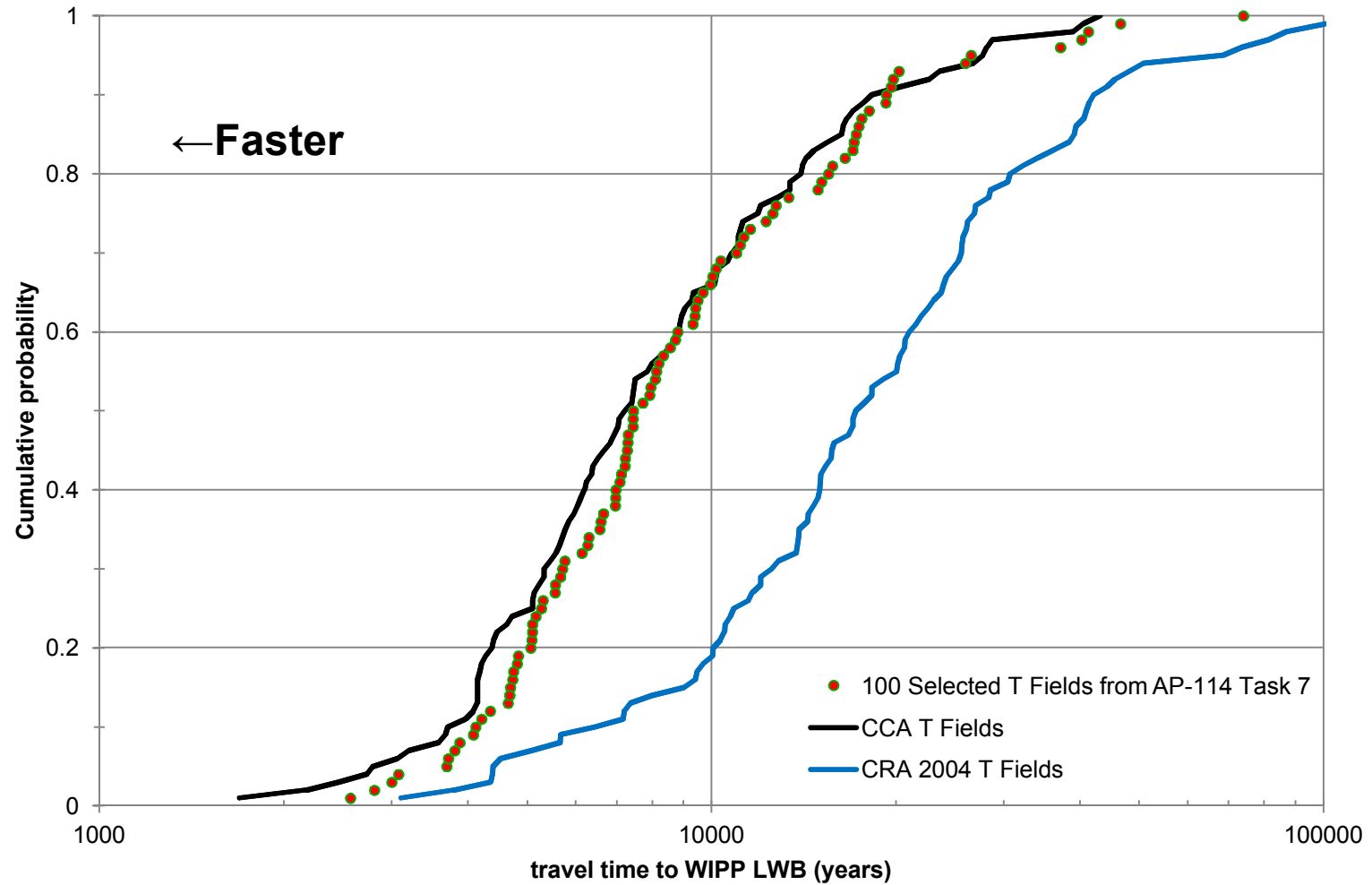
particles entire domain



Individual particle tracks inside LWB

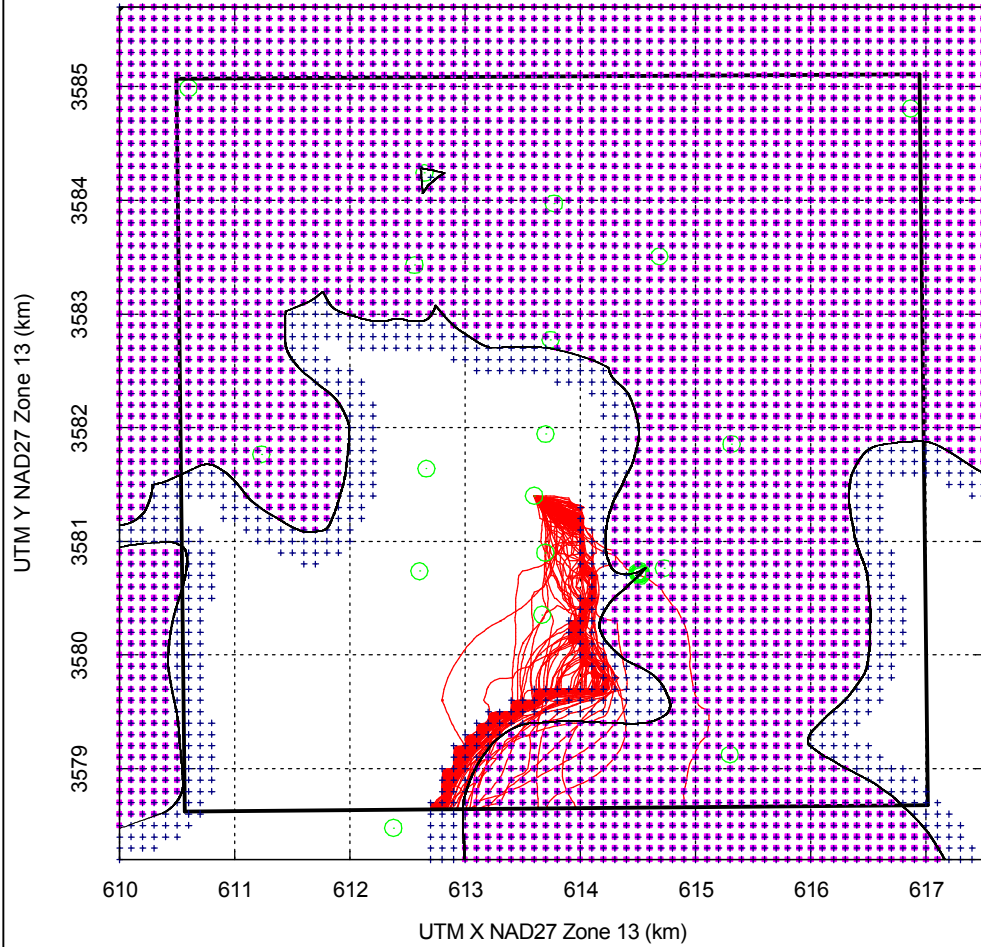


Particle Travel Times to WIPP LWB

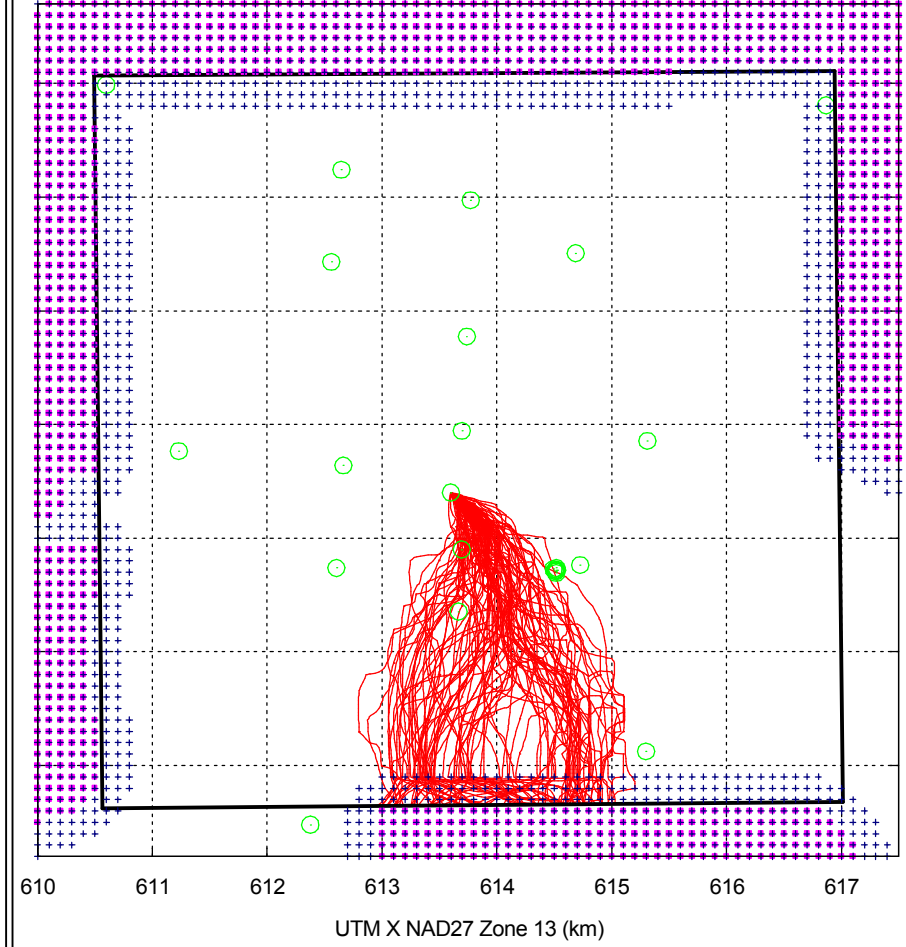


Particle Tracking

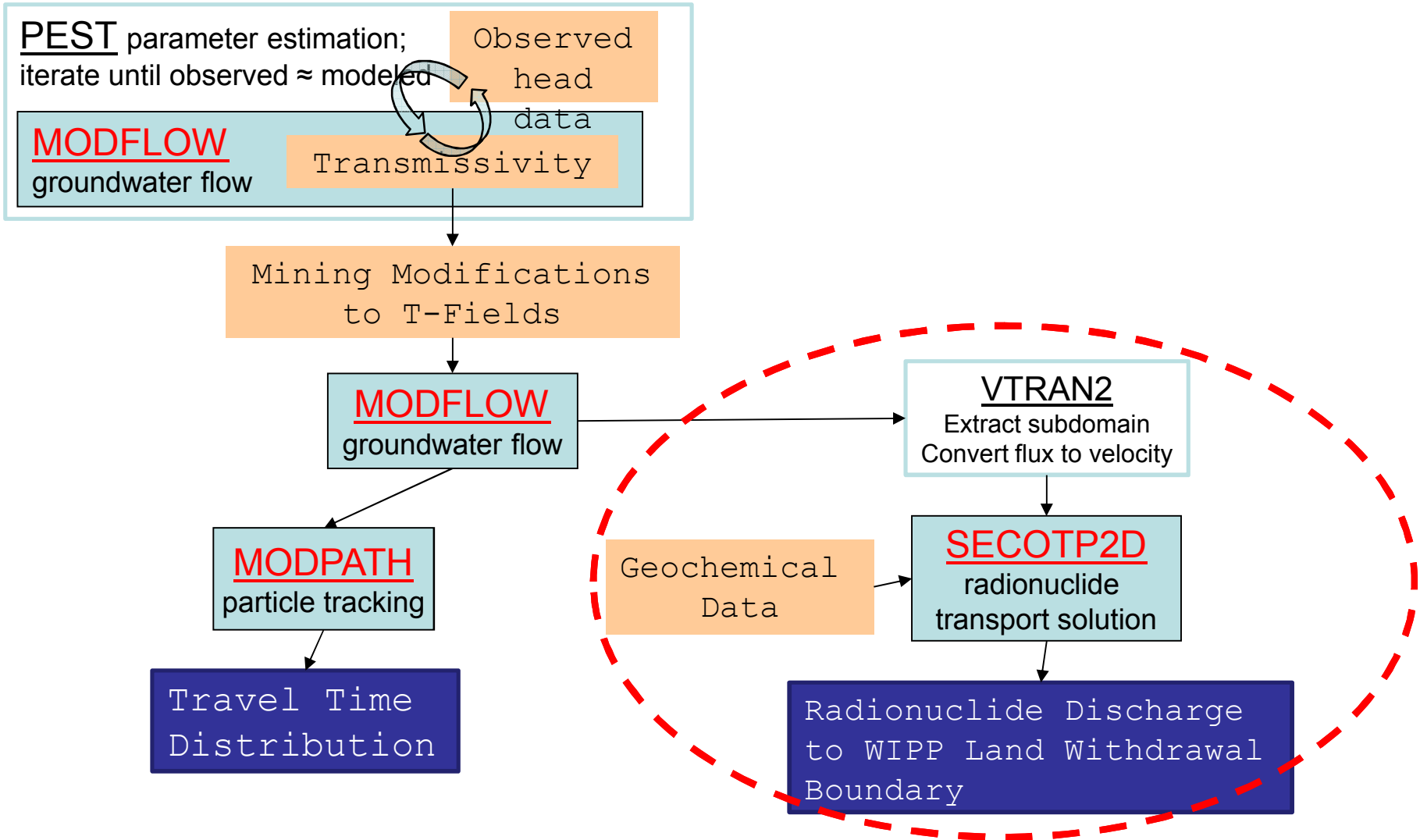
R1 full mining



R1 partial mining



Radionuclide Transport



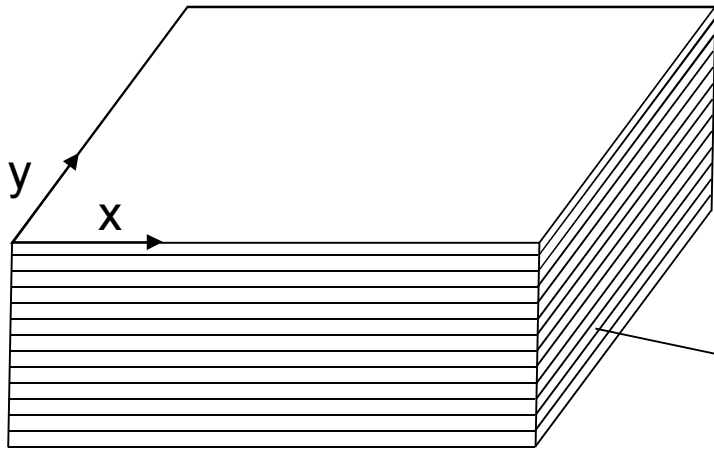
Transport Simulations

- Calculate transport of ^{241}Am , ^{239}Pu , ^{230}Th , ^{234}U
- Americium present as Am(III)
- Plutonium present as PU(III) or PU(IV)
- Thorium present as Th(IV)
- Uranium present as U(IV) or U(VI)
- 10,000 year interval
- Source at center of Waste Panel Area (WPA) injects 1kg total of each radionuclide during the interval [0,50 yr]
- Track cumulative releases across WPA and Land Withdrawal Boundary (LWB)

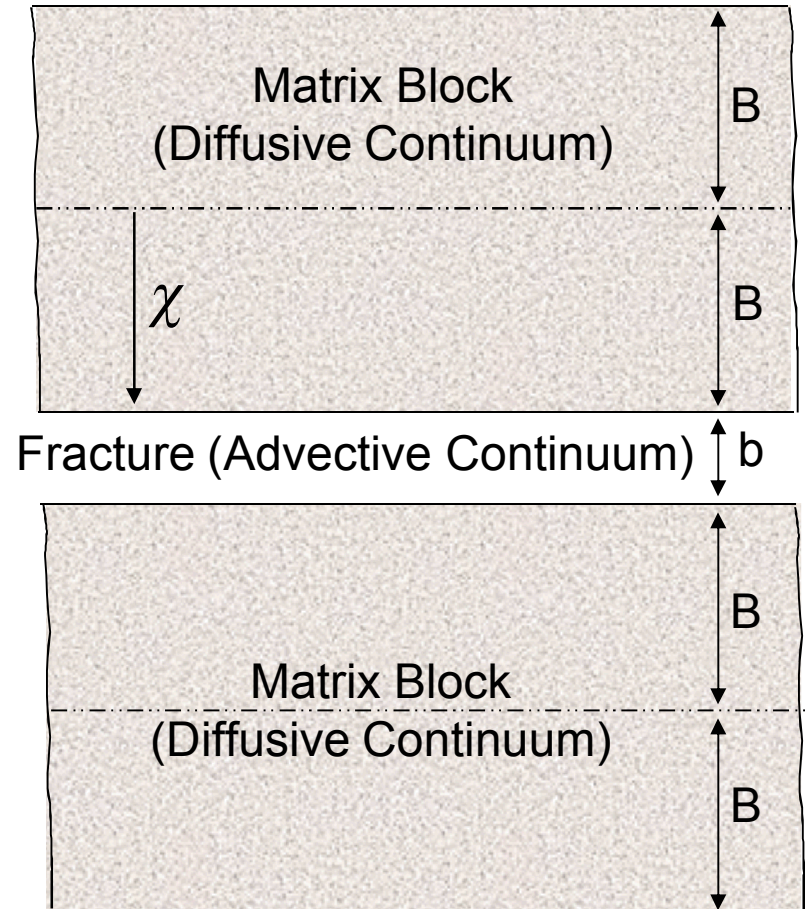
Transport Code (SECOTP2D)

- Three-level implicit temporal discretization
- Staggered finite volume mesh
- TVD advection scheme (advective continuum)
- Centered discretization of dispersion and diffusion terms
- Dimensional splitting
- Approximate factorization
- Implicit treatment of coupling term

SECOTP2D Dual Porosity Conceptualization



Planar Fracturing



Dual Domain Transport Equations

advective continuum equation for species $i = 1, \dots, N_{\text{species}}$,

$$\phi R_i \frac{\partial C_i}{\partial t} = \nabla \cdot (\phi \tau D_i^* \nabla C_i - \mathbf{V} C_i) - \phi R_i \lambda_i C_i + \underbrace{\phi R_{i-1} \lambda_{i-1} C_{i-1}}_{\text{daughter source}} + \Gamma_i$$

retardation for linear isotherm $R_i = 1 + \rho_s K_d^i \frac{1-\phi}{\phi}$

diffusive continuum equation (primed means diffusive domain)

$$\phi' R'_i \frac{\partial C'_i}{\partial t} - \frac{\partial}{\partial \chi} \left[\phi' \tau' D_i^* \frac{\partial C'_i}{\partial \chi} \right] = -\phi' R'_i C'_i + \underbrace{\phi' R'_{i-1} \lambda_{i-1} C'_{i-1}}_{\text{daughter source}}$$

mass-transfer equation between continua

$$\Gamma_i = -\frac{2\phi}{b} \left[\phi' D_i^* \frac{\partial C'_i}{\partial \chi} \Big|_{\chi=B} \right]$$

C_i	concentration	[M/L ³]
ϕ	advective porosity	[-]
\mathbf{V}	Darcy velocity vector	[L ² /T]
τ_i	advective tortuosity	[-]
D_i^*	free-water molecular diffusion	[L ² /T]
λ_i	radiactive species decay constant	[1/T]
χ	spatial block coordinate ($0 \leq \chi \leq B$)	[L]
K_d^i	distribution coefficient	[L ³ /M]

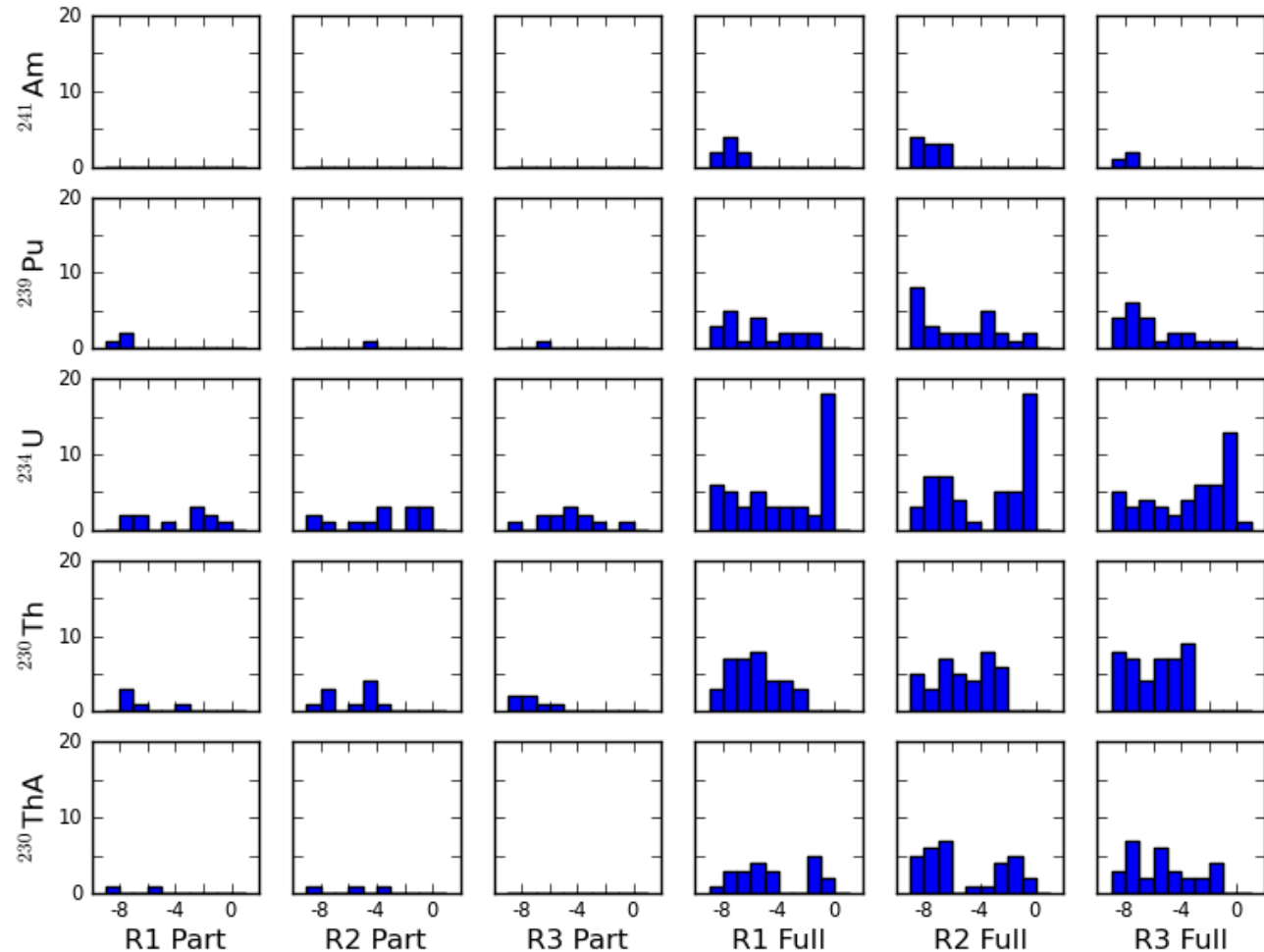
Transport Results

Histograms of radionuclide reaching LWB (cumulative over 10,000 years).

Releases greater than 10^{-9} kg shown (1kg injected total)

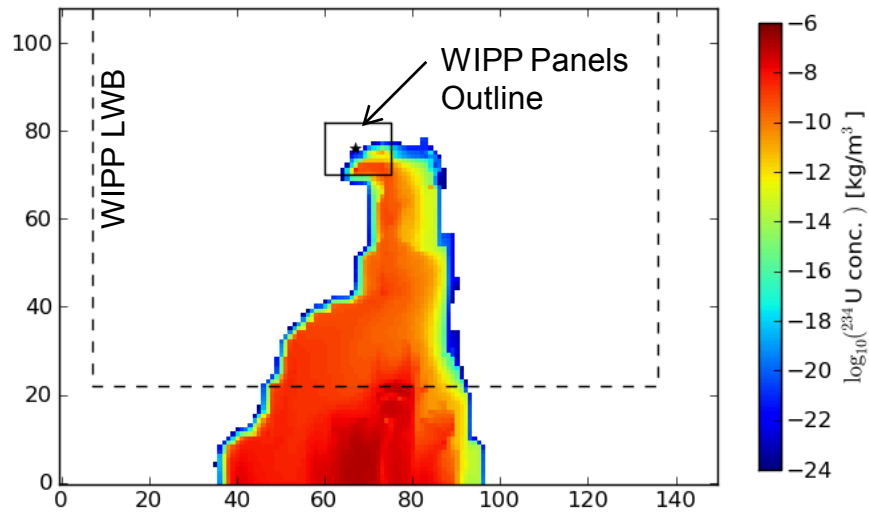
x-axes are \log_{10} concentration

y-axes are frequency (out of maximum possible 100)

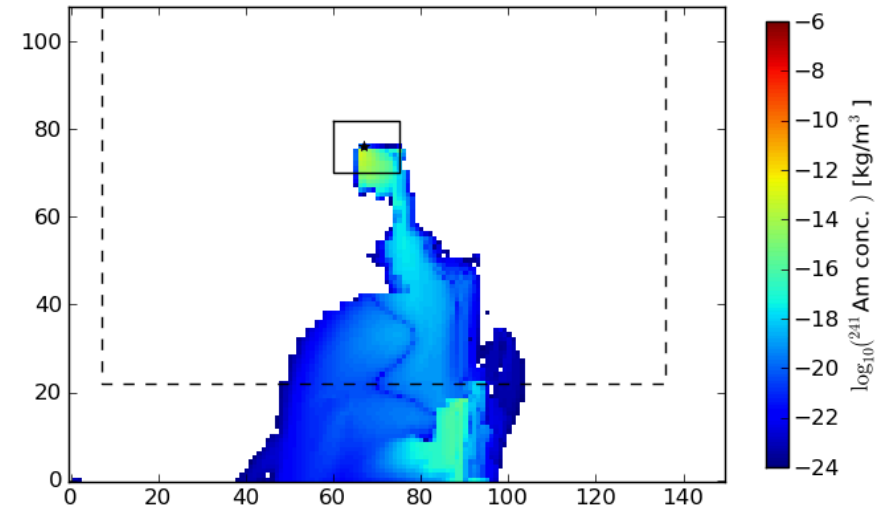


Transport Results: Largest Breakthrough Vectors

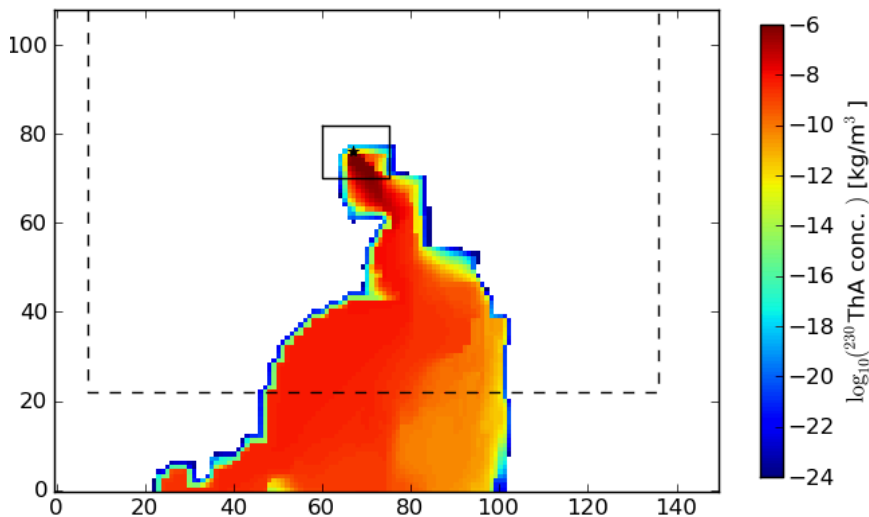
^{234}U R3 Full Mining V036



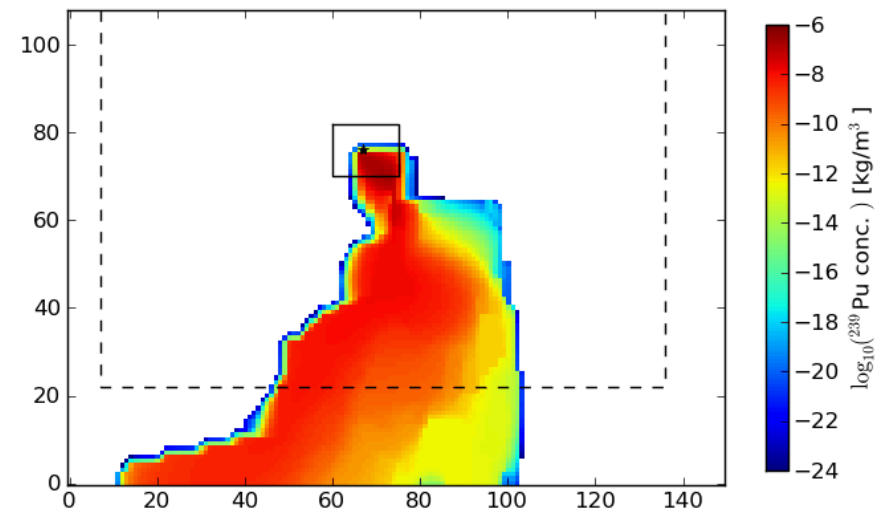
^{241}Am R2 Full Mining V099



^{230}ThA R1 Full Mining V098



^{239}Pu R2 Full Mining V050



References

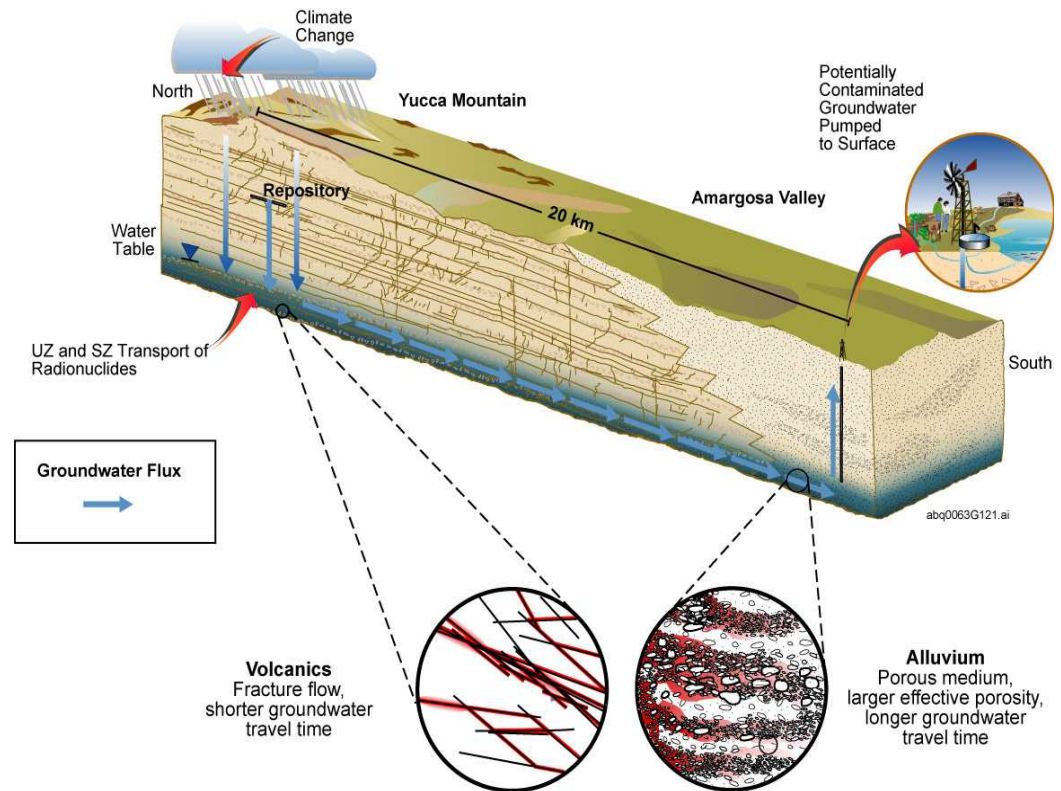
- Beauheim, R.L., 2008. *Analysis Plan for Evaluation and Recalibration of Cuelbra Transmissivity Fields AP-114, Revision 1*. Carlsbad, NM: Sandia National Laboratories.
- Hart, D.B., Beauheim, R.L. and McKenna, S.A., 2009. *Analysis Report for Task 7 of AP-114: Calibration of Culebra Transmissivity Fields*. Carlsbad, NM: Sandia National Laboratories. ERMS 552391.
- Hart, D.B., Holt, R.M. and McKenna, S.A., 2008. *Analysis Report for Task 5 of AP-114: Generation of Revised Base Transmissivity Fields*. Carlsbad, NM: Sandia National Laboratories. ERMS 549597.
- Holt, R.M. and Powers, D.W., 1988. *Facies variability and post-depositional alteration within the Rustler Formation in the vicinity of the Waste Isolation Pilot Plant, southeastern New Mexico*. Carlsbad, NM: Department of Energy. WIPP-DOE-88-004.
- Kirchner, T.B., 2010. *Sensitivity of the CRA-2009 Performance Assessment Baseline Calculation Releases to Parameters*. Carlsbad, NM: Sandia National Laboratories. ERMS 552960.
- Kuhlman, K.L., 2010a. *Analysis Report for the CRA-2009 PABC Culebra Flow and Transport Calculations (AP-144)*. Carlsbad, NM: Sandia National Laboratories. ERMS 552951.
- Kuhlman, K.L., 2010b. *Development of Culebra T-Fields for CRA-2009 PABC*. Carlsbad, NM: Sandia National Laboratories. ERMS 553276.
- Powers, D.W., 2007. *Analysis Report for Task 1A of AP-114: Refinement of Rustler Halite Margins Within the Culebra Modeling Domain*. Carlsbad, NM: Sandia National Laboratories. ERMS 547559.

Conceptual Model for Transport

The conceptual model for radionuclide transport varies with location in the saturated zone.

A dual porosity conceptual model of transport is used in the fractured volcanic units.

A porous medium conceptual model is used in the alluvium.



Upscaling of K_d Distributions

- Sorption coefficients were measured on *devitrified* and *zeolitic* tuff samples from the Yucca Mountain area for the radionuclides americium, barium, cesium, neptunium, plutonium, protactinium, radium, strontium, thorium, and uranium
- Data and analyses were used to obtain uncertainty distributions for the sorption coefficients
- Measurements represent a spatial scale on the order of centimeters
- A geostatistics-based scaling procedure was used to obtain from these distributions the uncertainty distributions on the scale of 500 m

Upscaling of K_d Distributions

- A stochastic approach was used to calculate effective values of K_d for a 500-m grid block
- The 500-m block was subdivided to the scale of 4 m
- Spatial distributions of rock type (either zeolitic or devitrified) at the 4m scale were generated using sequential indicator simulations (SIS)

Rock type distribution: 1, 0, 1, 1, 1, 0, 0, ..., 1

- Using SIS and the observed K_d data, spatially heterogeneous realizations of K_d at a scale of 4 m for each rock type were developed

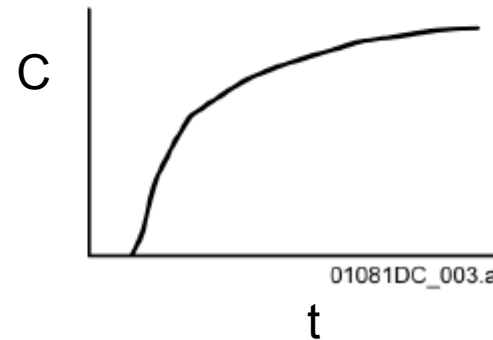
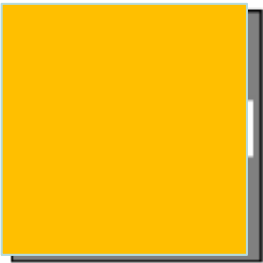
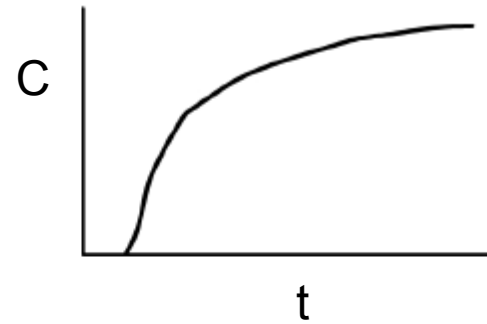
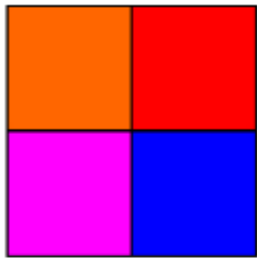
K_d distribution for rock type '1': $K_{d1}^1, K_{d2}^1, K_{d3}^1, K_{d4}^1, K_{d5}^1, K_{d6}^1, K_{d7}^1, \dots, K_{dn}^1$

K_d distribution for rock type '0': $K_{d1}^0, K_{d2}^0, K_{d3}^0, K_{d4}^0, K_{d5}^0, K_{d6}^0, K_{d7}^0, \dots, K_{dn}^0$

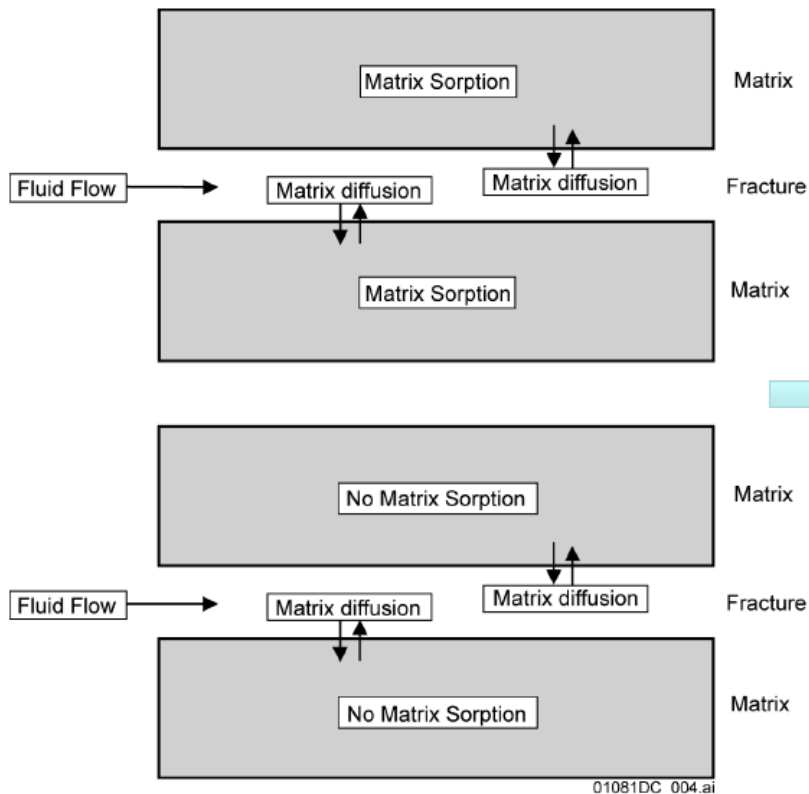
Combined K_d distribution: $K_{d1}^1, K_{d2}^0, K_{d3}^1, K_{d4}^1, K_{d5}^1, K_{d6}^0, K_{d7}^0, \dots, K_{dn}^1$

- Transport calculations used to determine effective K_d for 500-m grid block for each realization

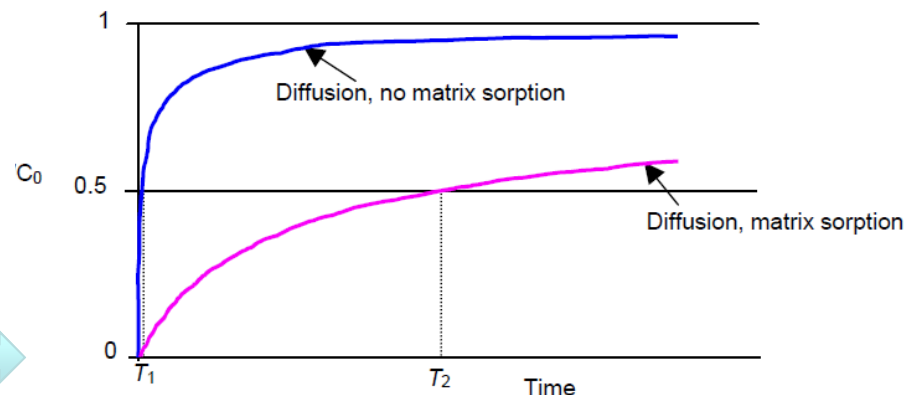
Schematic Representation of the Definition of Effective K_d



Effective Retardation and K_d



Processes during Transport of a Radionuclide in a Fractured Media



Representation of the Breakthrough Curves Used to Calculate Effective Matrix Retardation Behavior

$$\text{Effective Retardation } (r_{\text{eff}}) = \frac{T_2}{T_1}$$

$$K_d = (\text{retardation coeff.} - 1) \frac{\text{Porosity}}{\text{Bulk Density}}$$

Upscaled Effective K_d Values

Derived from Experimentally Observed K_d Values

Radionuclide	Rock-type	Distribution	Mean (mL/g)	Standard Deviation (mL/g)	Minimum (mL/g)	Maximum (mL/g)
Uranium	Zeolitic	Truncated Normal	12.0	3.6	5.0	20.0
	Devitrified	Truncated Normal	2.0	0.6	0.0	4.0
Cesium	Zeolitic	Exponential	16,942.0	14,930.0	4,000.0	42,000.0
	Devitrified	Truncated Normal	728.0	464.0	100.0	1,000.0
Neptunium	Zeolitic	Truncated Normal	2.88	1.47	0.0	6.0
	Devitrified	Exponential	0.69	0.71	0.0	2.0
Plutonium	Zeolitic	Beta	100.0	15.0	50.0	300.0
	Devitrified	Beta	100.0	15.0	50.0	300.0

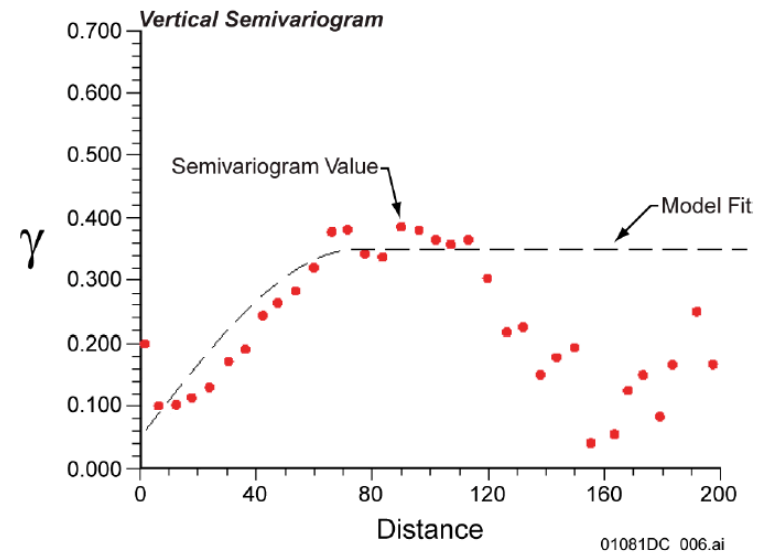
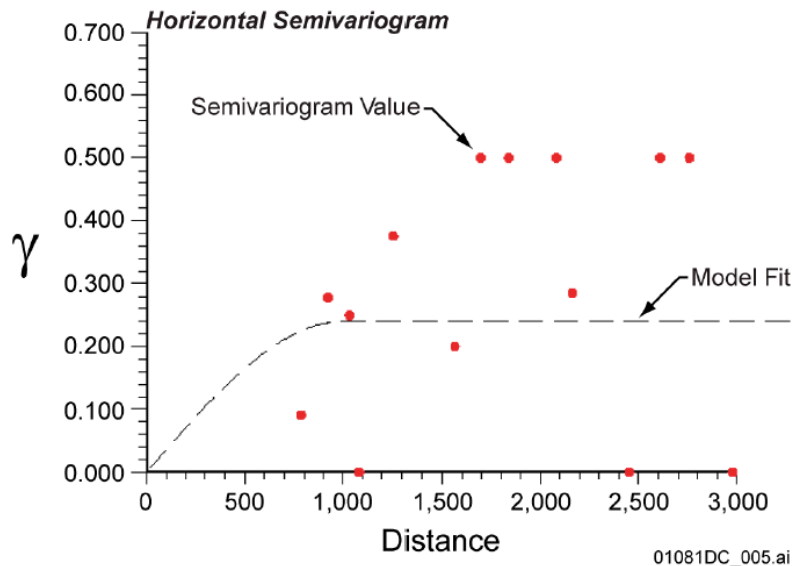


Upscaled Effective K_d Values

Radionuclide	Distribution	Mean	Standard Deviation	Minimum	Maximum
Uranium	Truncated Normal	6.61	0.61	5.39	8.16
Cesium	Truncated Normal	5,188.72	941.55	3,000.59	6,782.92
Plutonium	Truncated Normal	110.17	7.45	89.90	129.87
Neptunium	Truncated Normal	1.48	0.23	0.99	1.83

Steps in Upscaling

- Transform observed well data into indicator code
 - Two rock types – zeolitic and devitrified
 - $I = 1$ if zeolitic, $I = 0$ if devitrified
- Develop two directional indicator semivariograms



- Generate multiple realizations of spatial distribution of rock types

Steps in Upscaling

- After the spatial distributions of rock types were generated, the small scale distributions were used to generate realizations of *K_d values*
- Indicators were defined at four CDF cutoffs of 0.2, 0.4, 0.6, and 0.8 e.g., for U K_d (ml/g) is 8.97, 11.09, 12.91, 15.03, respectively
- These cutoffs, along with spatial correlation information, were then used to generate spatial distributions of *K_d* values for each rock type
- The rock type-specific *K_d* distributions and rock-type distributions were used to generate integrated *K_d* distributions
- Transport calculations were used to determine effective *K_d* for 500-m block

Upscaled Effective K_d Values

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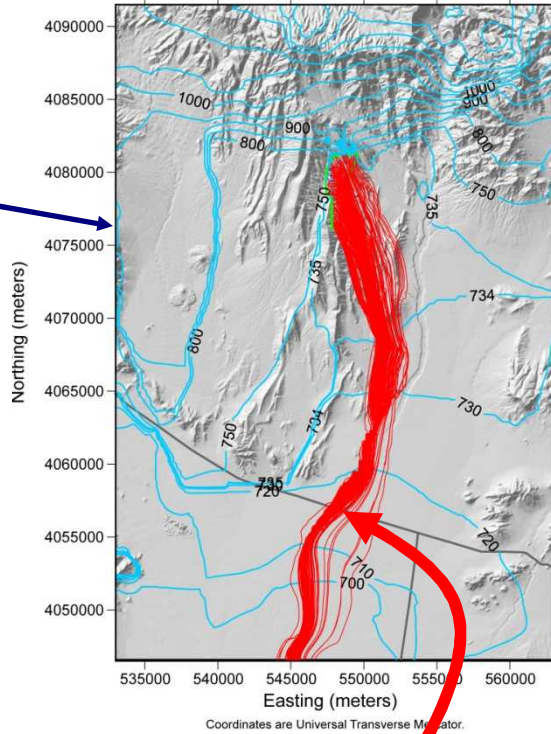
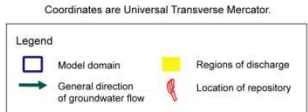
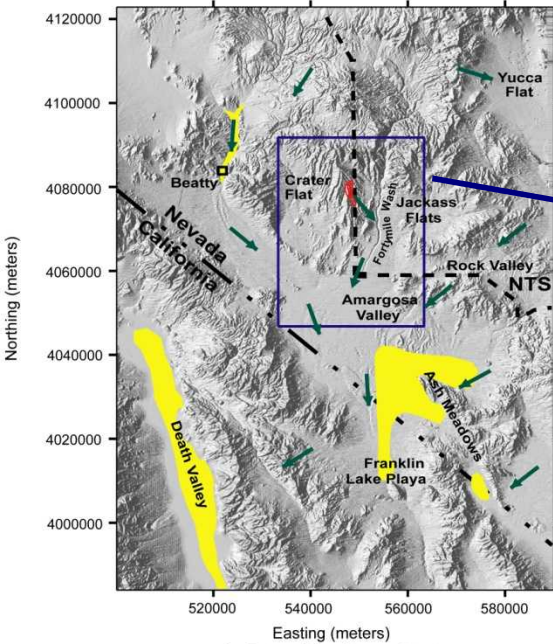
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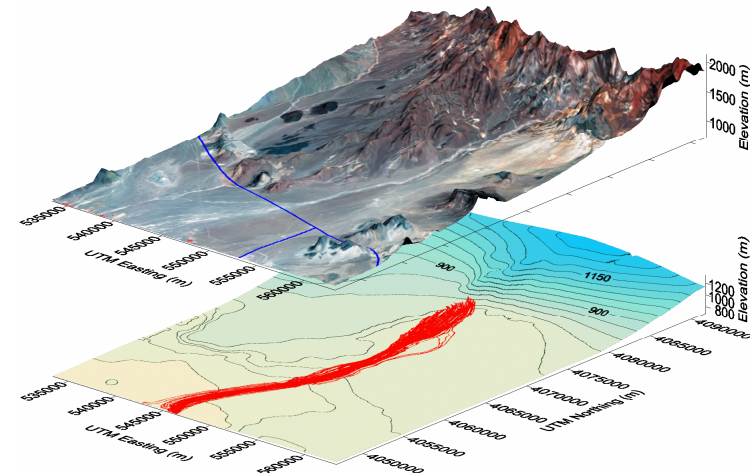
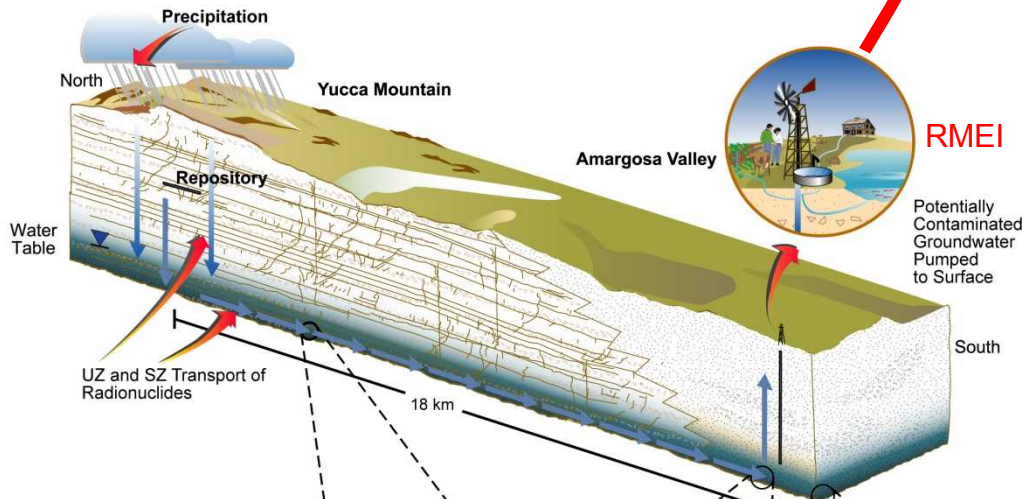
Parameter Uncertainties in the SZ

- Groundwater flow and geological uncertainty:
 - Groundwater specific discharge
 - Horizontal anisotropy in permeability (fractured tuff)
 - Alluvium – tuff contact in the subsurface
- Radionuclide transport uncertainty:
 - Matrix diffusion in fractured tuff
 - ◆ Flowing interval spacing
 - ◆ Effective diffusion coefficient in tuff matrix
 - ◆ Flow porosity in tuff
 - Sorption coefficients (tuff matrix and alluvium)
 - Dispersivity (longitudinal, transverse horizontal and vertical)
 - Effective porosity of alluvium
 - Source location
 - Colloid retardation factor (tuff and alluvium)
 - Sorption coefficients onto colloids
 - Groundwater colloid concentration

Saturated Zone Flow and Transport



- Particle tracking method includes radionuclide transport processes of advection, dispersion, matrix diffusion in fractured volcanic units, and sorption
- Simulated flow paths from the repository occur in the upper few hundred meters of the SZ



Summary of Key Points

Characterization of Uncertainty

- **Quantitative assessments of uncertainty in predictive performance assessments are important**
- **Quantifying and reducing conceptual model uncertainty is an important and challenging task**
- **Conceptual model uncertainty can be very difficult to identify, quantify, and assess**
- **In many cases, conceptual model uncertainty has larger impact on performance assessment and project costs than parameter uncertainty**
- **Conceptual model uncertainty is best addressed through experimental work and detailed process modeling**

Summary of Key Points

Coupling Site Characterization and Performance Assessment

- **Site characterization should be cautious about focusing attention on assumed dominant processes or pathways before performance assessment modeling is performed**
- **For experimental guidance, performance assessment should use reasonable estimates of parameter and conceptual uncertainty and not conservative assumptions that may bias results towards preconceived ideas**
- **Neither site characterization nor performance assessment should completely dominate iterative interactions**

Summary of Key Points

Technical Interactions Between Site Characterization and PA Staff

- **Formalized integration between site characterization and performance assessment groups can be facilitated through workshops on major system components**
- **Project management can enhance integration by encouraging collaboration between individual staff members from site characterization and performance assessment groups**
- **Mutual technical review of project documentation by site characterization and performance assessment groups contributes to information exchange and consistency**

Summary of Key Points

Uncertainty and Sensitivity Analysis

- **Both site characterization and performance assessment groups have important contributions to make to understanding uncertainty**
- **Uncertainty and sensitivity analyses at both the total system level and the sub-system model level provide insights about behavior of the repository system**
- **Involvement of both site characterization and performance assessment groups in uncertainty / sensitivity analyses and prioritization decisions can contribute to consensus regarding project direction**

Summary of Key Points

- **Projects begin with a broad-based approach to site characterization (SC) to identify site features relevant to performance**
- **Once initial site characterization has been completed, a FEPs (Features, Events, and Processes) analysis can be performed**
- **FEPs analysis can focus future work on the features of the repository environment and the physical/chemical processes of greatest importance to PA**

Summary of Key Points

- **Early PA and FEPs results should not be used to terminate experimental programs on the grounds that safety can be adequately demonstrated without invoking the process or mechanism to be studied**
- **Early understandings of the relative importance of different processes sometimes change as a project progresses, and no real barrier to radionuclide migration should be ignored simply because it “isn’t needed” nor should less likely pathways be ignored because a dominant pathway can be “conservatively” assumed**

Summary of Key Points

- **The first groundwater flow models developed showed that a high-transmissivity region in the Culebra dolomite, thought to be bounded on all sides, actually continued off-site and would be the dominant flow pathway**
- **Additional field work was performed to refine our knowledge of the extent and hydraulic properties of this zone**

Summary of Key Points

PA Guidance for SC

- **A sensitivity analysis is performed for every PA that is completed to identify the uncertain (sampled) parameters having the largest effects on calculated releases**
- **If additional experimentation could reduce the range of uncertainty of the sensitive parameters, more tests may be performed**
- **SC and PA continue in an iterative fashion**

Summary of Key Points

Limitations of PA

- **PA can only show the relative importance of parameters in the context of the models it is employing – if the models are inadequate or inappropriate, unsound guidance may be provided to SC**
- **Additional SC may identify the need for alternative models**

Summary of Key Points

- **SC and PA should evolve together through an iterative process, with neither activity completely dominating the other**
- **For experimental guidance, PA should use reasonable estimates of parameter and conceptual uncertainty, and not conservative assumptions that may bias results towards preconceived notions**
- **SC should be cautious about focusing attention too much on assumed dominant processes or pathways before PA modeling is performed**

Summary of Key Points

Defensibility and Credibility

- **Models must always be appropriate to the scale of test or investigation**
- **Using more detailed models for test interpretation than can/will be used in PA:**
 - **allows a detailed understanding of a process to be developed and demonstrated a defensible basis for model simplification as the scale of interest increases**

Summary of Key Points

- **Double-porosity models with multirate diffusion have been used to model tracer-test results from the Culebra to demonstrate understanding of the important processes, even though a model using a single rate of diffusion may be suitable for PA**
- **Use of a simplified model in PA has not been challenged because of the underlying detailed understanding**

Summary of Key Points

Safety Case

- **“A Safety Case is the synthesis of evidence, analyses and arguments that quantify and substantiate a claim that the repository will be safe after closure and beyond the time when active control of the facility can be relied on.” (OECD NEA, 2004)**
- **Safety cases involve both quantitative (e.g., PA) and qualitative (e.g., reasoned arguments) elements**

Summary of Key Points

- **SC provides hard data to be used in PA calculations as well as the conceptual understanding of the site that is needed to develop a safety case**
- **SC must provide a convincing description of parts of the overall system not explicitly included in PA models**
- **SC Support of the Safety Case**

Summary of Key Points

- **Defensibility and credibility require a much greater depth of understanding than can be represented in PA models**



SC must go beyond the needs of PA to support the overall Safety Case

Summary of Key Points

- **SC and PA typically occur simultaneously, with the result that different people are responsible for each**
- **Model simplification, however, requires an understanding of how processes operate at both the experimental and PA scales**
- **At WIPP and YMP, experimentalists were not willing to defend PA models and parameters until they were directly involved in developing the models and selecting parameter values**
Model/Parameter Abstraction

Summary of Key Points

- **Experimentalists should be directly involved in model and parameter abstraction and simplification for PA**

Summary of Key Points

- **Site characterization and PA should evolve together through an iterative process, with neither activity completely dominating the other**
- **Early PA and FEPs results should not be used to terminate experimental programs on the grounds that safety can be adequately demonstrated without invoking the process or mechanism to be studied**

Summary of Key Points

- **Prioritization of additional work must balance the factors of performance assessment sensitivity, costs, trade-offs in uncertainty and design, and qualitative political or social considerations.**
- **Integration among site characterization, repository design, and performance assessment groups is important to successful and acceptable prioritization efforts.**

Summary of Key Points

- *There may be important trade-offs between reduction in uncertainty and control of the system through repository design modifications.*
- *Alternative repository design features may be able to compensate for uncertainty in the system (e.g., YMP drip shields and uncertainty in drift seepage).*
- *Some alternative repository design features included to improve performance may actually increase uncertainty in the system (e.g., YMP high-temperature waste loading and coupled hydrothermal processes).*

Summary of Key Points

- **Factors other than the quantitative sensitivity of the PA model may be important to consider in the prioritization of data collection and analyses.**
- **Public and political confidence in the repository system may require a minimum level of understanding for certain aspects of the system, regardless of the expected quantitative impact on performance.**
- **Some data collection tasks that have a high technical priority may also require long time frames, placing them in conflict with project schedule goals.**

Summary of Key Points

- **Intermediate priority is placed on activities that would result in large reductions in uncertainty in an important aspect of the system at a relatively high cost and activities that would result in modest reductions in uncertainty at a low cost.**
- **Formal quantitative methods of decision analysis exist for calculating the value of information associated with additional site characterization.**
- **Decisions on project priorities may be complicated by qualitative considerations.**

Summary of Key Points

- **Prioritization of site characterization activities should be based primarily on quantitative information obtained through assessment of uncertainties, modeling and sensitivity analysis.**
- **Actual decisions regarding additional data collection and analyses must also consider the costs associated with obtaining those data.**
- **Highest priority is placed on activities that would result in large reductions in uncertainty in an important aspect of the system at a relatively low cost.**