SAND2007-6831P

Groundwater Flow and Radionuclide Transport Modeling in WIPP Performance Assessment

KHNP Training Program
Module 6: Assembly of a Safety Case

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Outline

I. Introduction: Groundwater Flow and Radionuclide Transport in WIPP PA

II. Description of Conceptual Models

   A. Groundwater Flow

   B. Radionuclide Transport

III. Numerical Implementation

   A. T-Field Calibration

   B. Mining Modifications

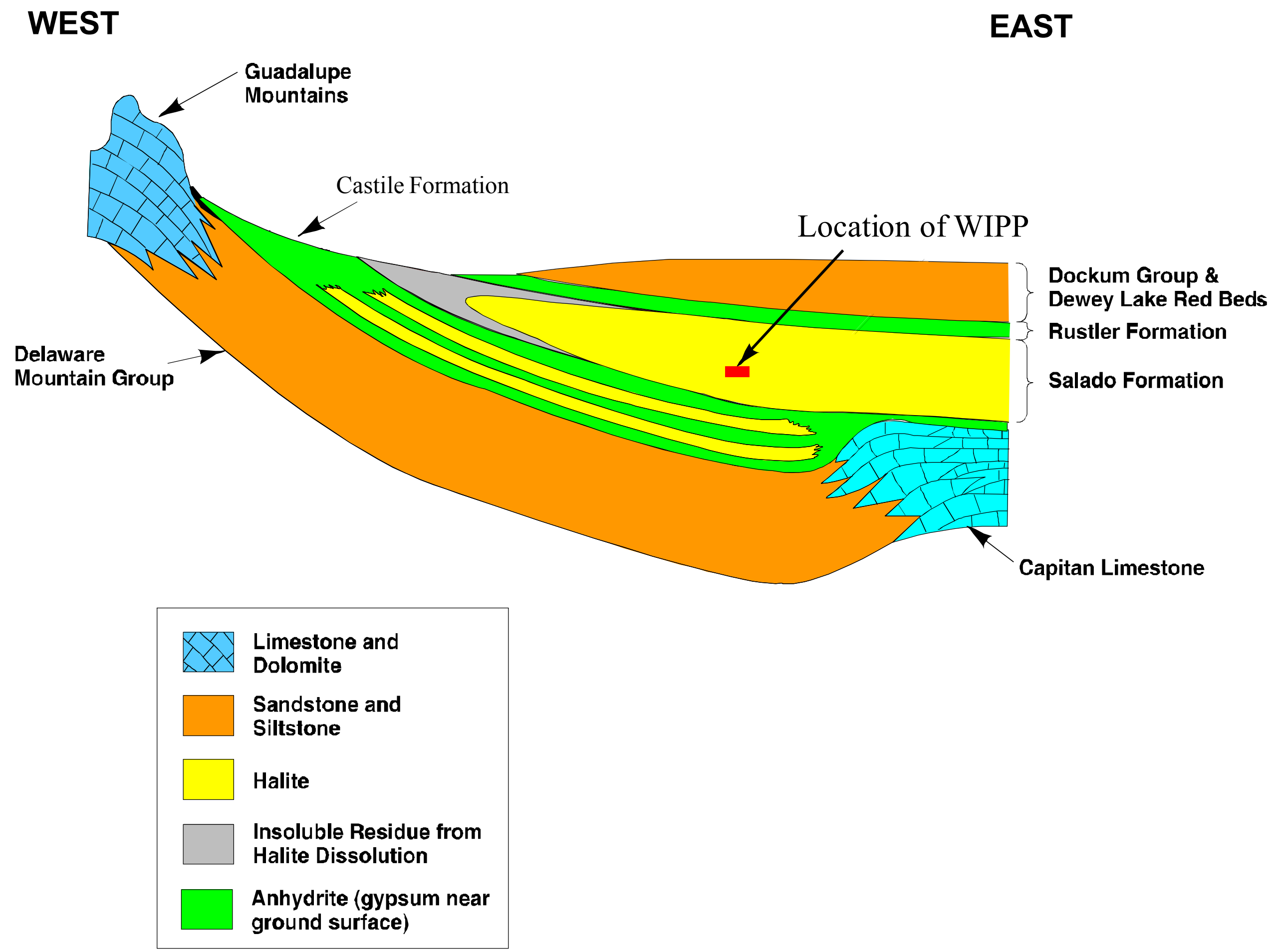
   C. Flow Calculations

   D. Transport Calculations

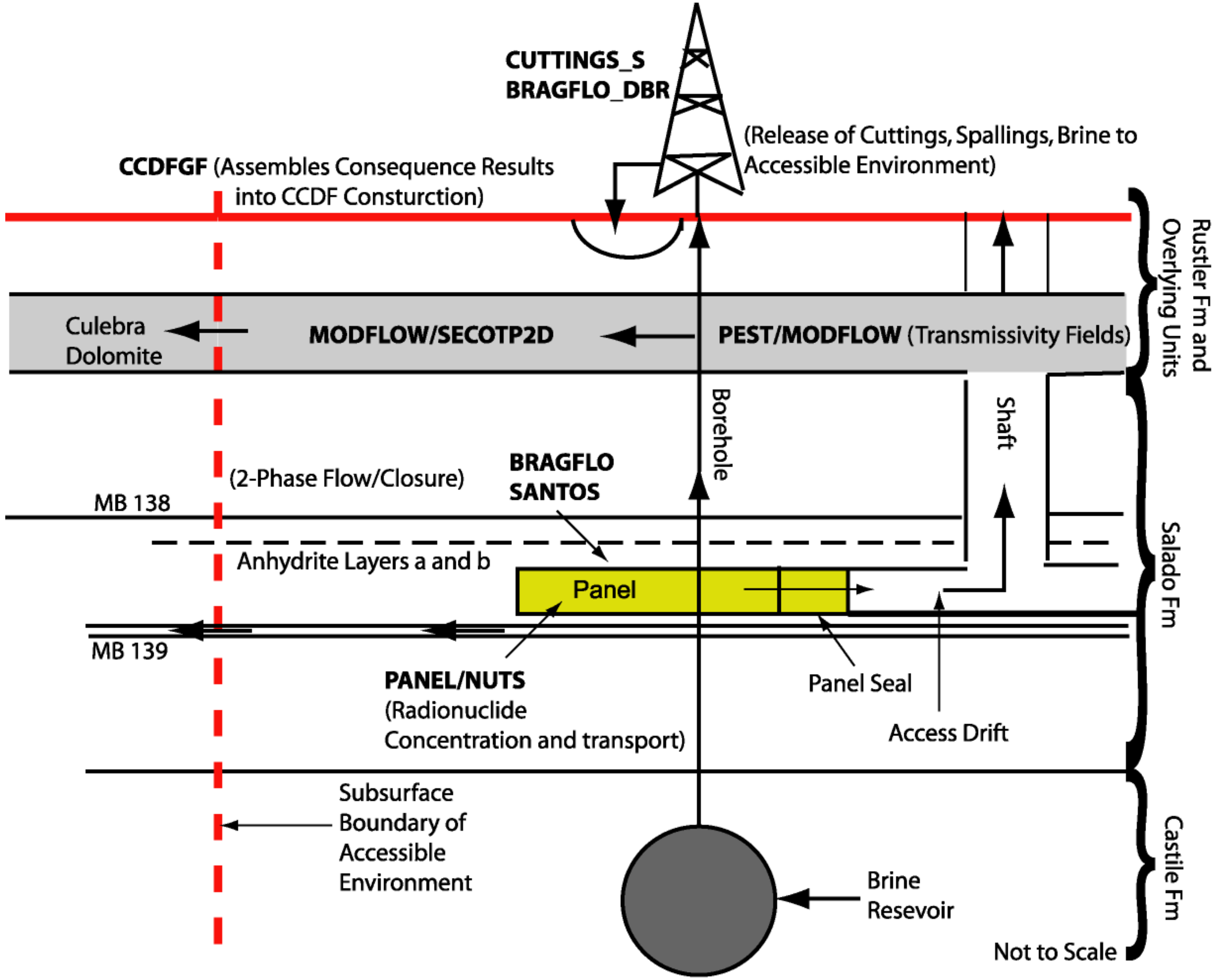
IV. Results

Introduction

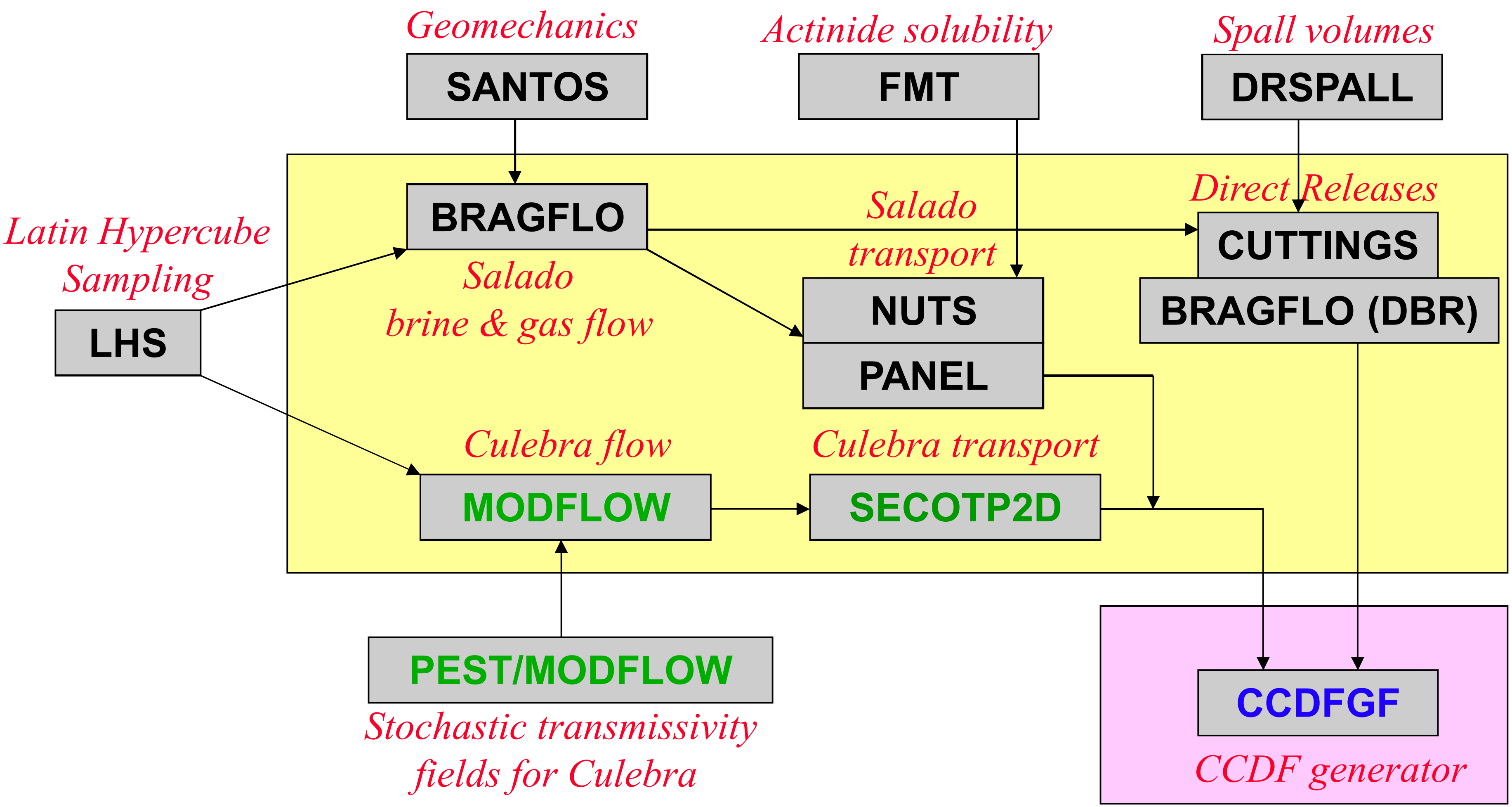
Stratigraphy in WIPP Vicinity



Release Pathways

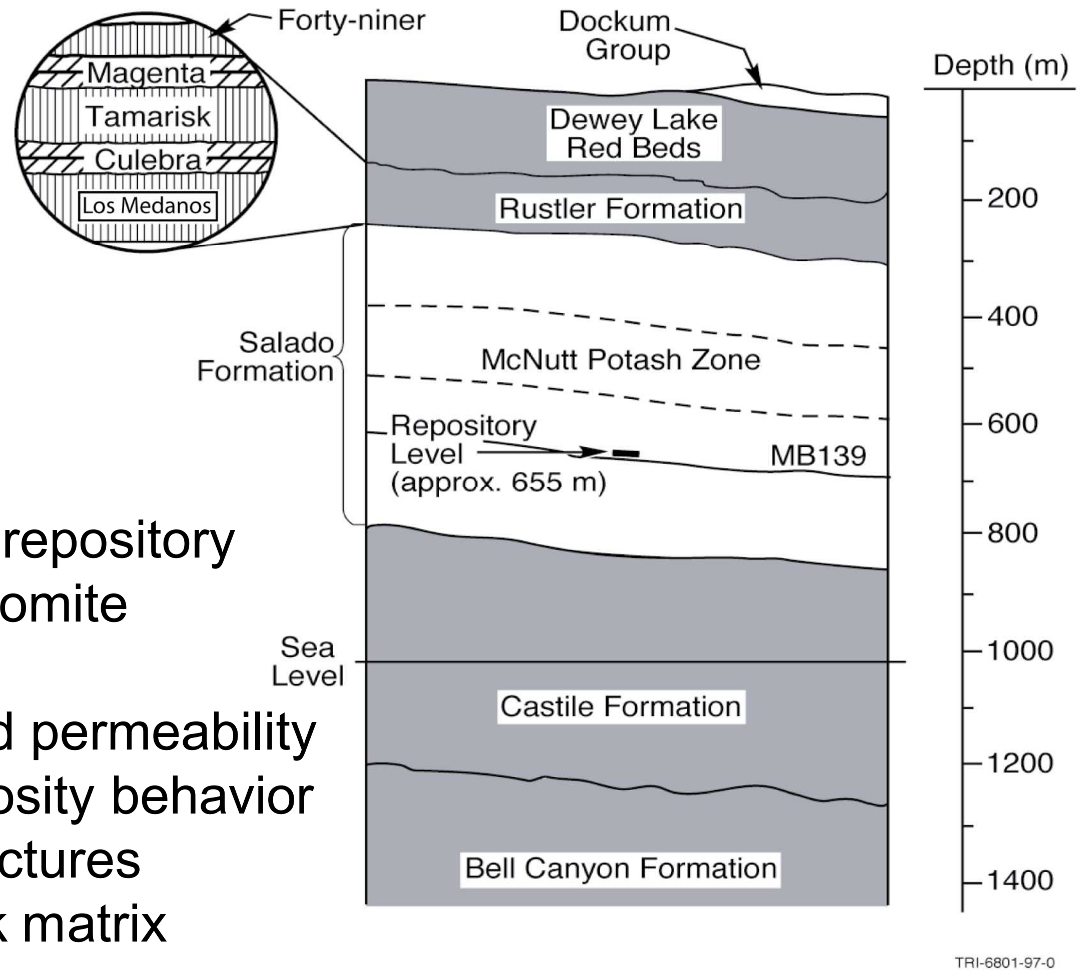


Major WIPP PA Simulation Codes



Conceptual Models

Rustler Formation in WIPP Vicinity

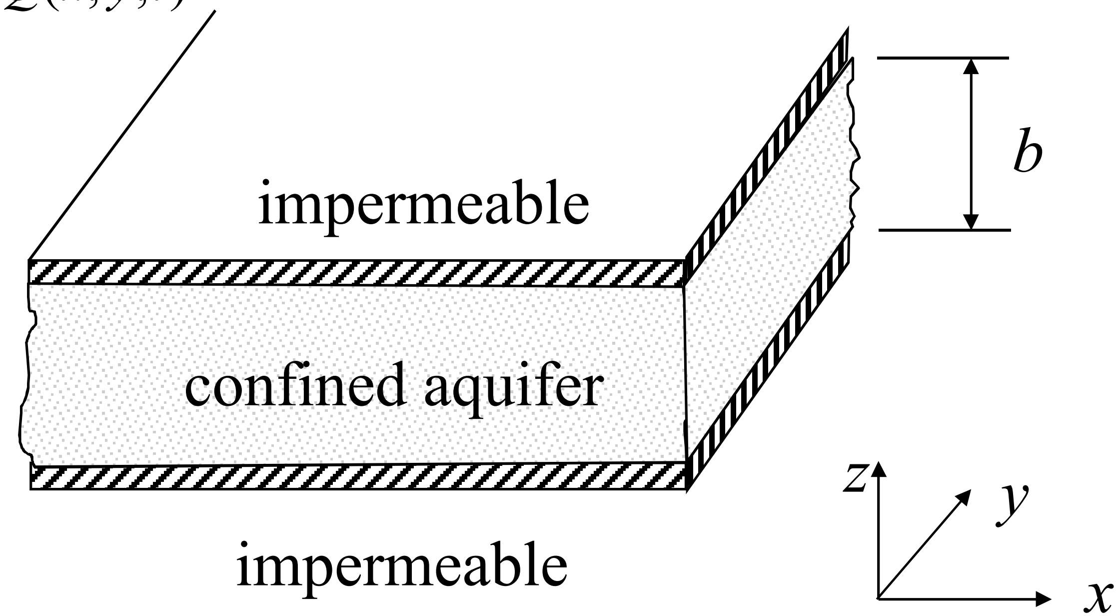


<u>Culebra Formation</u>

- Most transmissive unit above repository
- 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

2-D Groundwater Flow

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



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

$T = Kb$

where:

$\phi \equiv$ potentiomteric head [L]

z $\equiv$ elevation [L]

p $\equiv$ pressure [$ML^{-1}T^{-2}$]

$\gamma \equiv$ specific weight of water [$ML^{2}T^{2}$]

$S \equiv$ aquifer storativty [-]

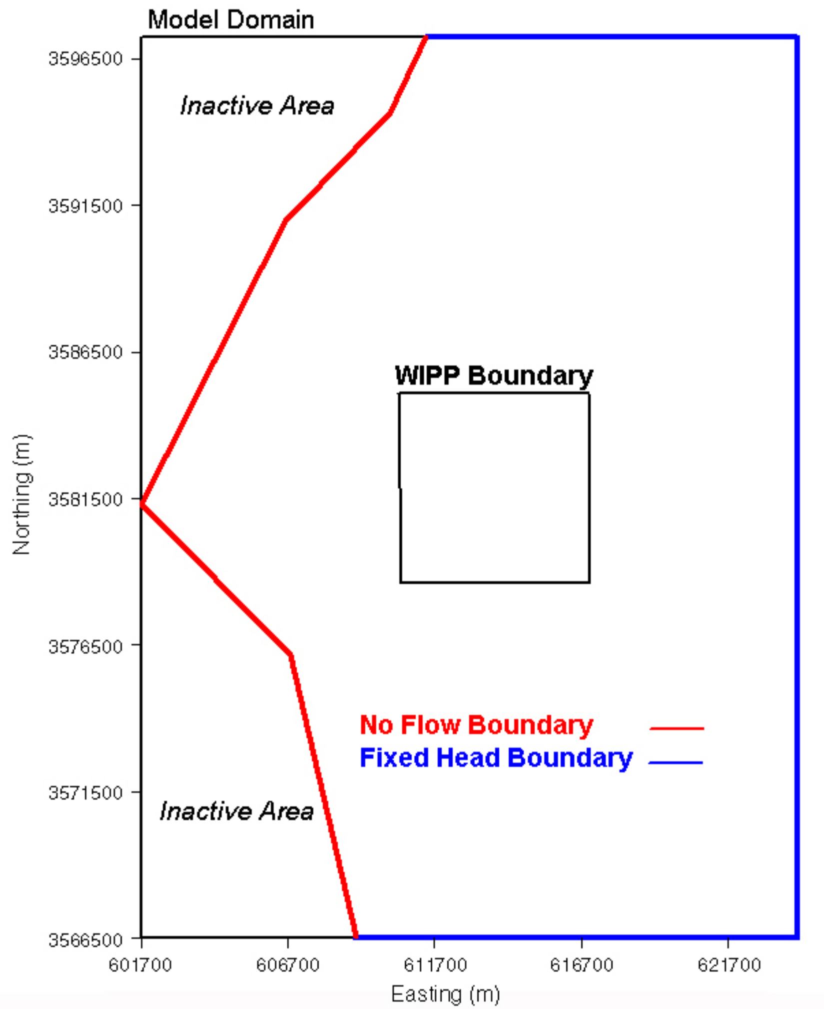
T $\equiv$ aquifer transmissivity [$L^{2}T^{-1}$]

K $\equiv$ hydraulic conductivity [LT^{-1}]

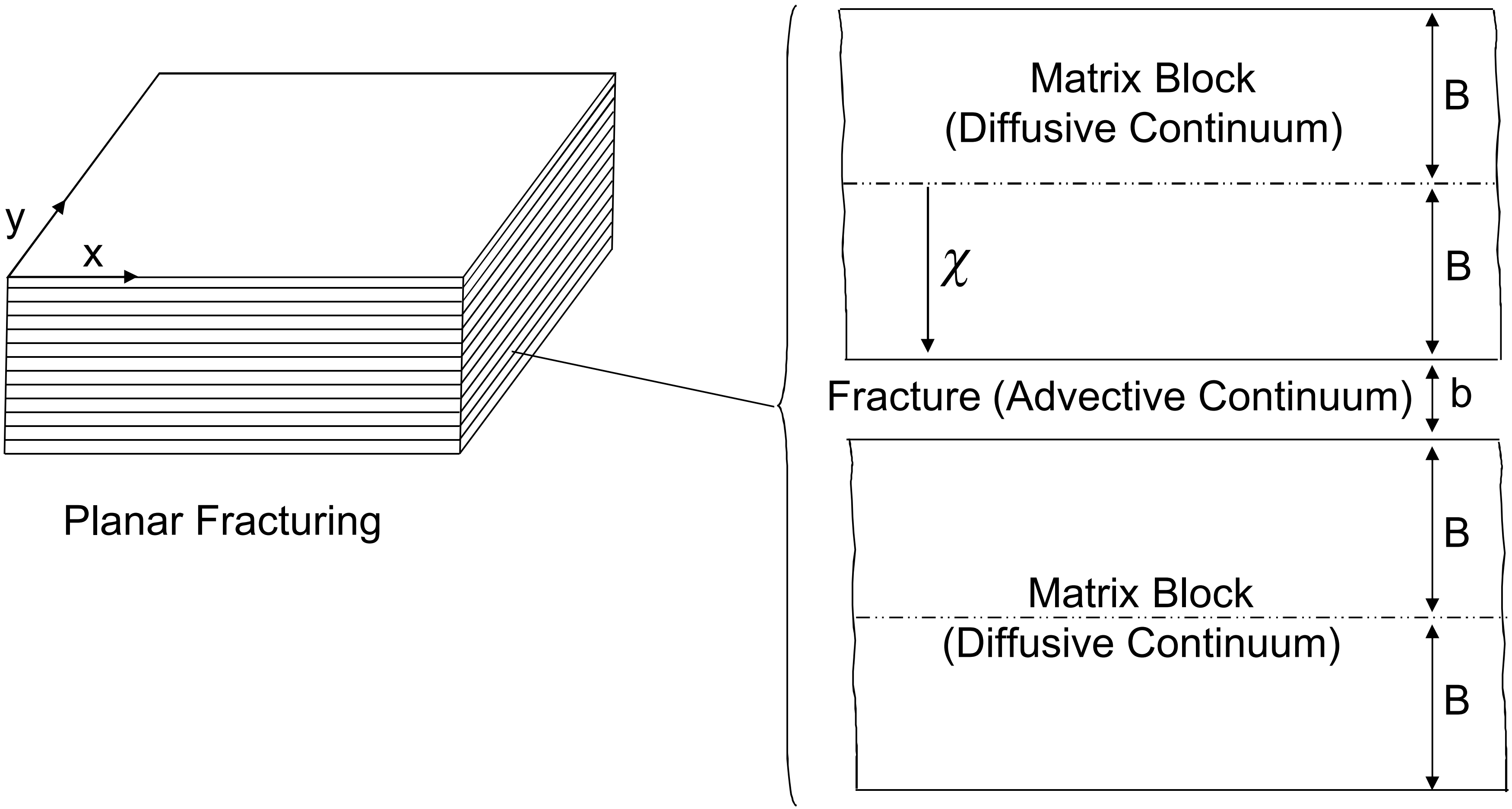
$b \equiv$ aquifer thickness [L]

$Q \equiv$ source/sink per unit area $\left[LT^{-1}\right]$

Groundwater Modeling Domain and Boundary Conditions



Dual Porosity Conceptualization



Planar Fracturing

Advective Continuum Governing Equation

$$\phi R_k \frac{\partial C_k}{\partial t} = -\nabla \bullet \left(\mathbf{v} C_k \right) + \nabla \bullet \left(\phi \mathbf{D}_k \nabla C_k \right) - \phi R_k \lambda_k C_k + \phi R_{k-1} \lambda_{k-1} C_{k-1} + Q_k + \Gamma_k$$

$$\phi D_k = \frac{1}{|\mathbf{v}|} \begin{bmatrix} u & -v \\ v & u \end{bmatrix} \begin{bmatrix} \alpha_L & 0 \\ 0 & \alpha_T \end{bmatrix} \begin{bmatrix} u & v \\ -v & u \end{bmatrix} + \phi \tau D_k^*$$

$$R_k = 1 + \frac{\rho_s \left(1 - \phi\right) \left(K_d\right)_k}{\phi}$$

Diffusive Continuum Governing Equation

$$\phi^{'} R_k^{'} \frac{\partial C_k^{'}}{\partial t} = \frac{\partial}{\partial \chi}\left(\phi^{'} D_k^{'} \frac{\partial C_k^{'}}{\partial \chi} \right) - \phi^{'} R_k^{'} \lambda_k C_k^{'} + \phi^{'} R_{k-1}^{'} \lambda_{k-1} C_{k-1}^{'}$$

$$D_k^{'} = \tau D_k^{*}$$

$$R_k^{'} = 1 + \frac{\rho_s \left(1 - \phi^{'}\right)\left(K_d^{'}\right)_k}{\phi^{'}}$$

Coupling Term

$$\Gamma_k = -\frac{2\phi}{b}\left(\phi^{'} D_k^{'} \left[\frac{\partial C_k^{'}}{\partial \chi}\right]_{\chi = B}\right)$$

$$b = \frac{\phi B}{1 - \phi}$$

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Initial and Boundary Conditions

Initial Conditions

$$C_k\left(x,y,0\right)=0 \quad \forall\left(x,y\right)\in\Omega$$

$$C_k^{'}\left(\chi,0\right)=0 \quad \forall\left(\chi\right)\in\Omega^{'}$$

Boundary Conditions

$$C_k\left(x,y,t\right)=0 \quad \left|\partial\Omega\bullet\mathbf{v}\right|<0, \quad \forall t>0$$

$$\left[\frac{\partial C_k}{\partial n}\right]_{\partial\Omega}=0 \quad \left|\partial\Omega\bullet\mathbf{v}\right|\geq 0, \quad \forall t>0$$

$$\left[C_k^{'}\left(B,t\right)\right]_{(x,y)}=C_k^{'}\left(x,y,t\right), \quad \forall t>0$$

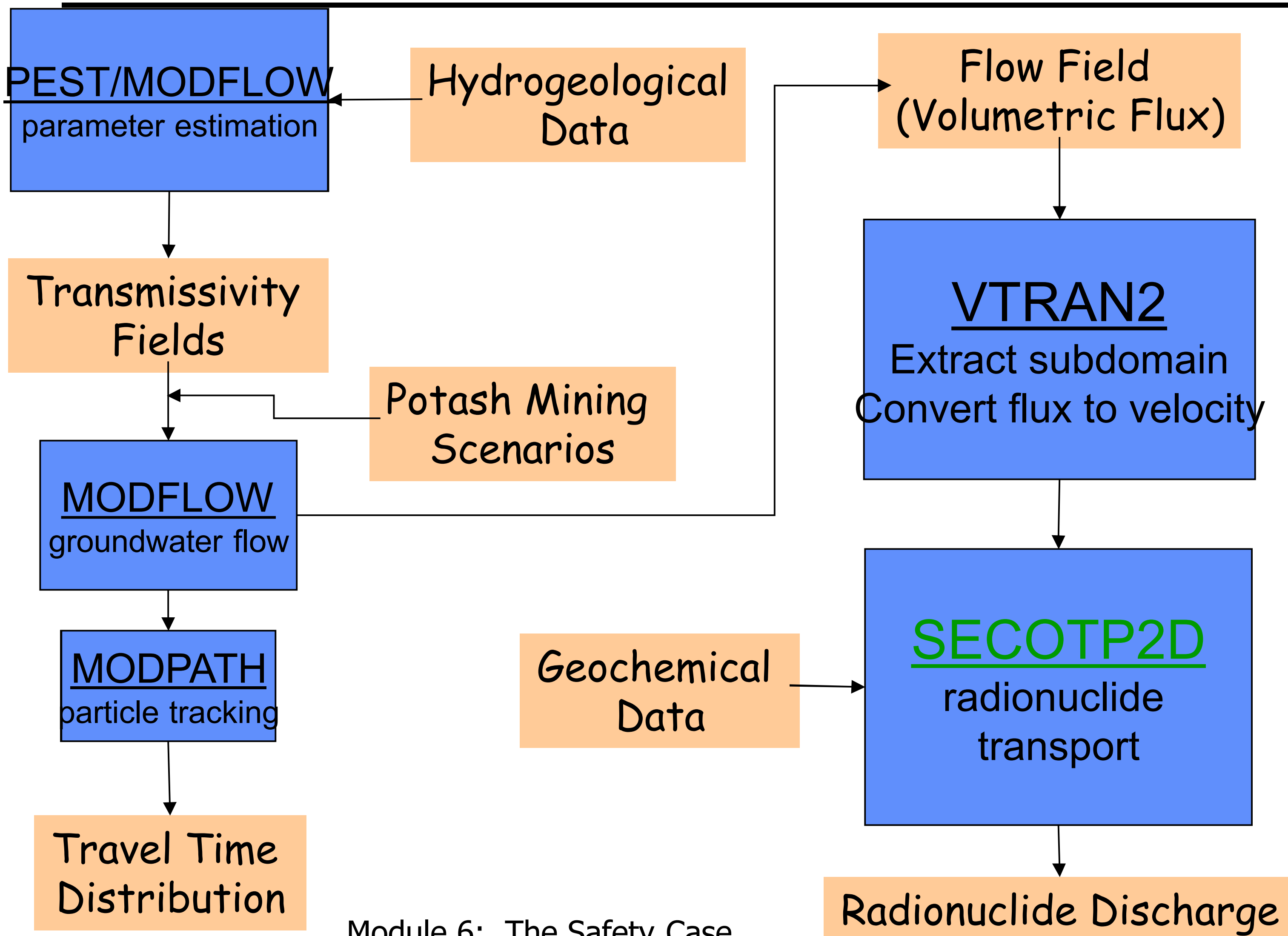
$$\left[\frac{\partial C_k^{'}}{\partial\chi}\right]_{\chi=0}=0, \quad \forall t>0$$

Numerical Implementation

Steps in Numerical Impementation

- T-Field Calibration
- Mining Modifications
- Flow Calculations
- Transport Calculations

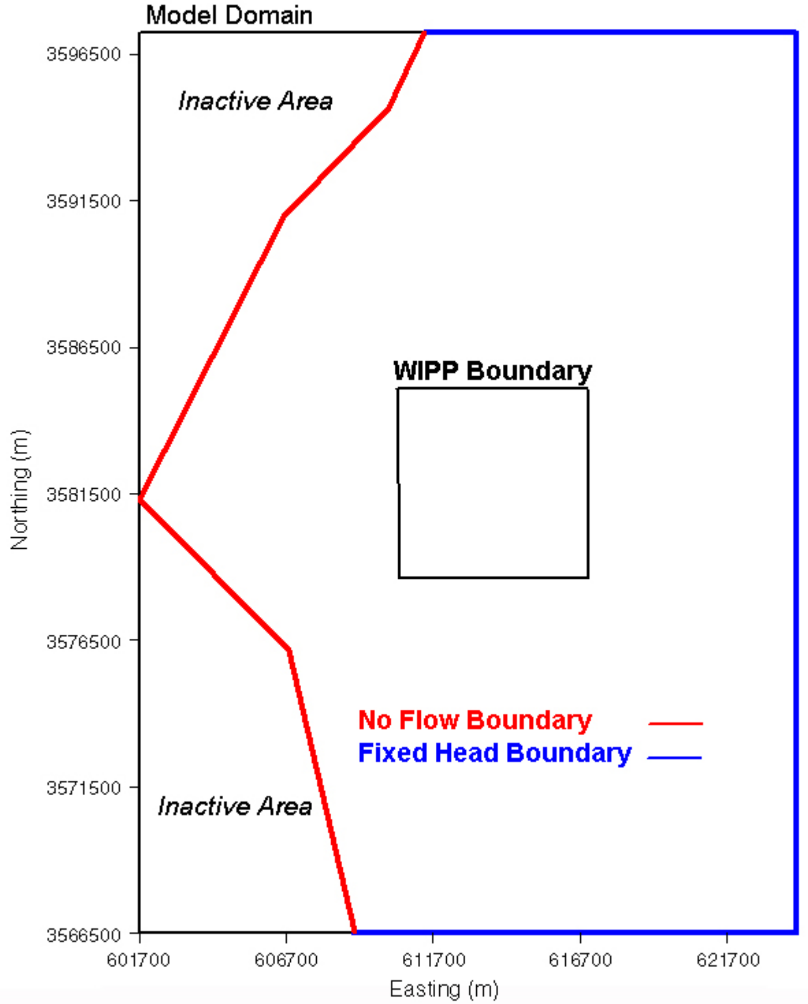
Culebra Flow and Transport Calculation Flowchart



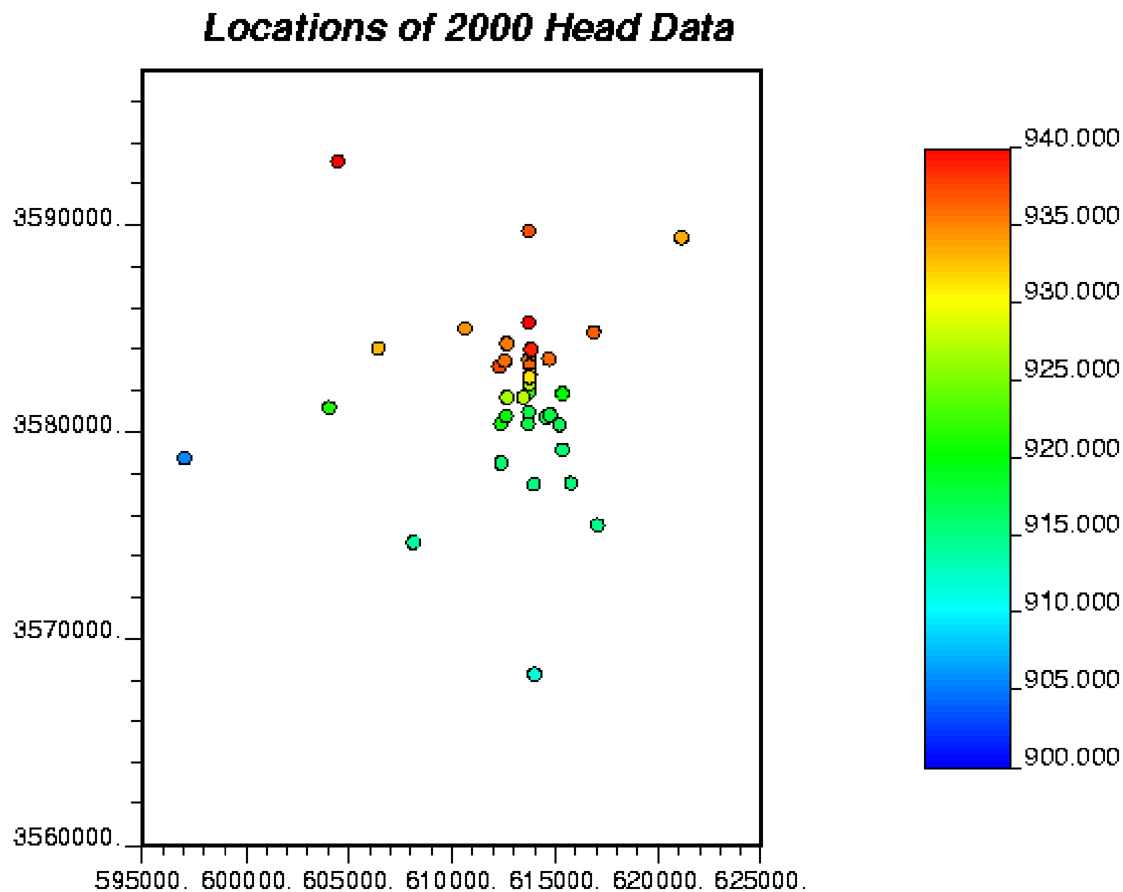
T-Field Calibration

Boundary Conditions

- Interpolating/extrapolating the observed heads to the boundary cells
- Estimated heads provide fixed head values for boundary cells and initial heads for model
- Kriging used to estimate heads at all cells
- Use trend removal prior to kriging



2000 Steady-State Head Data



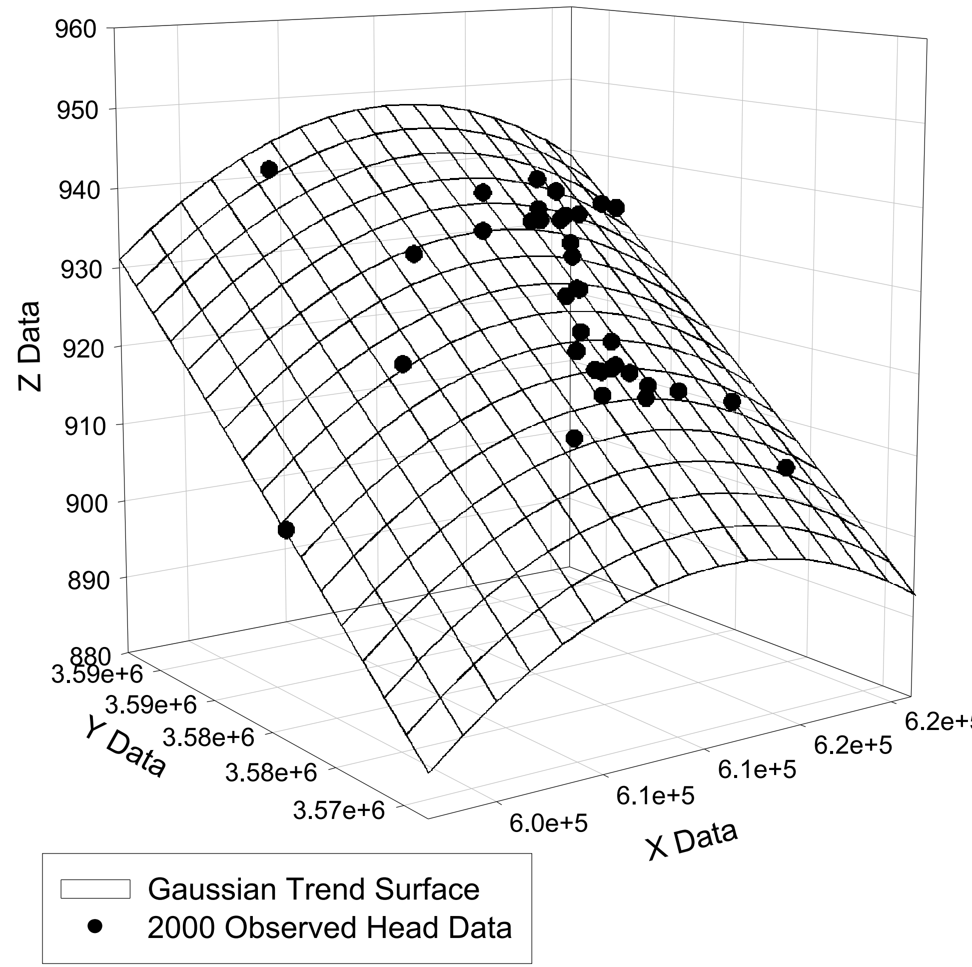
Black rectangle denotes flow model domain

Trend Removal

- Fit bivariate Gaussian surface to observed head data
- Calculate residuals as:
  - Residual head = (observed head) - (bivariate Gaussian surface)
- Calculate and model spatial correlation of residuals (variogram)
- Estimate residuals across site (kriging)
- Add residuals to the bivariate Gaussian surface to get head estimates

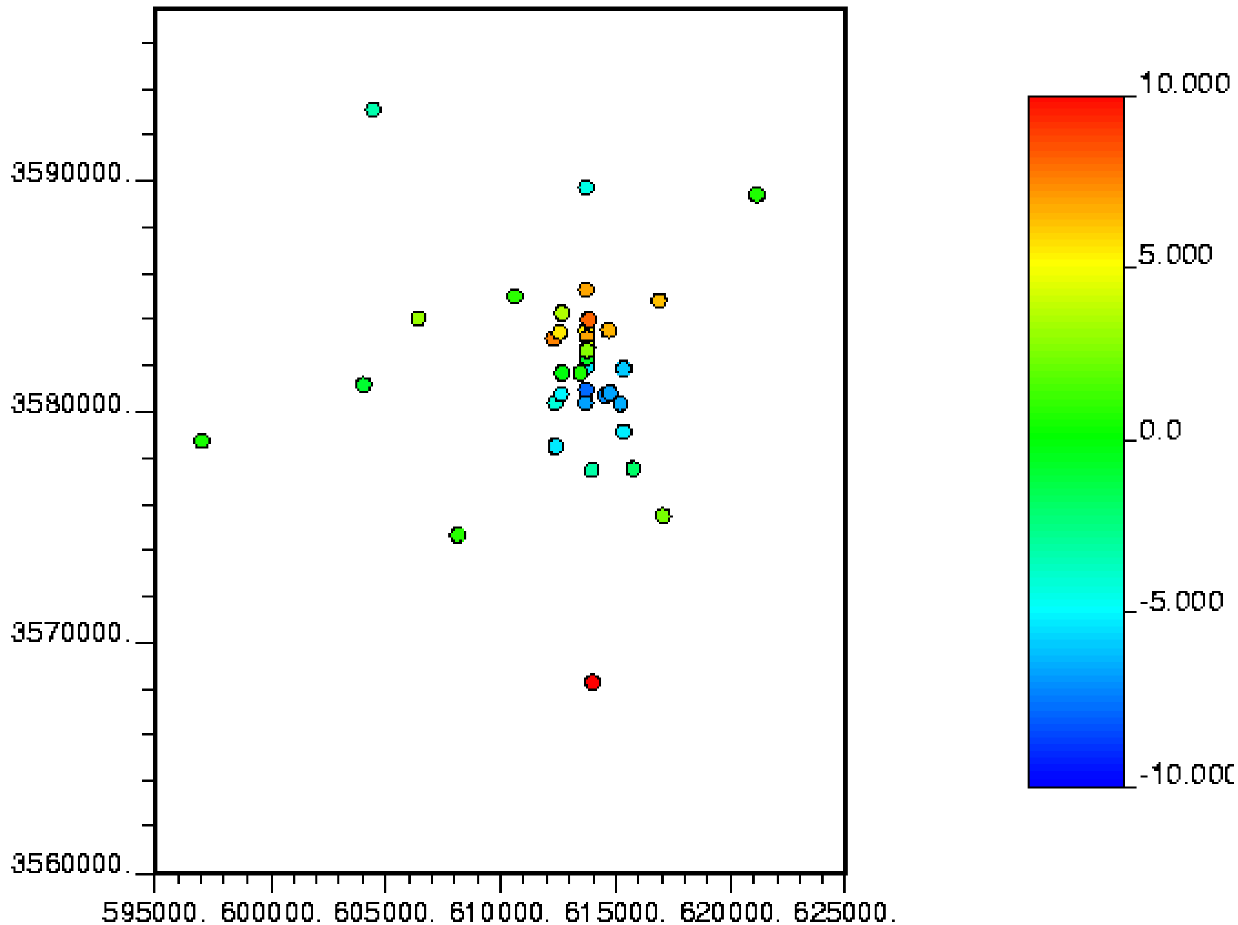
Head Trend Surfaces

- **Bivariate Gaussian trend surface is fit to the heads**
- **Can be difficult to fit all heads to the surface (e.g., H-9b and H-10b)**



Head Residuals

Residuals between the bivariate Gaussian surface and the observed heads



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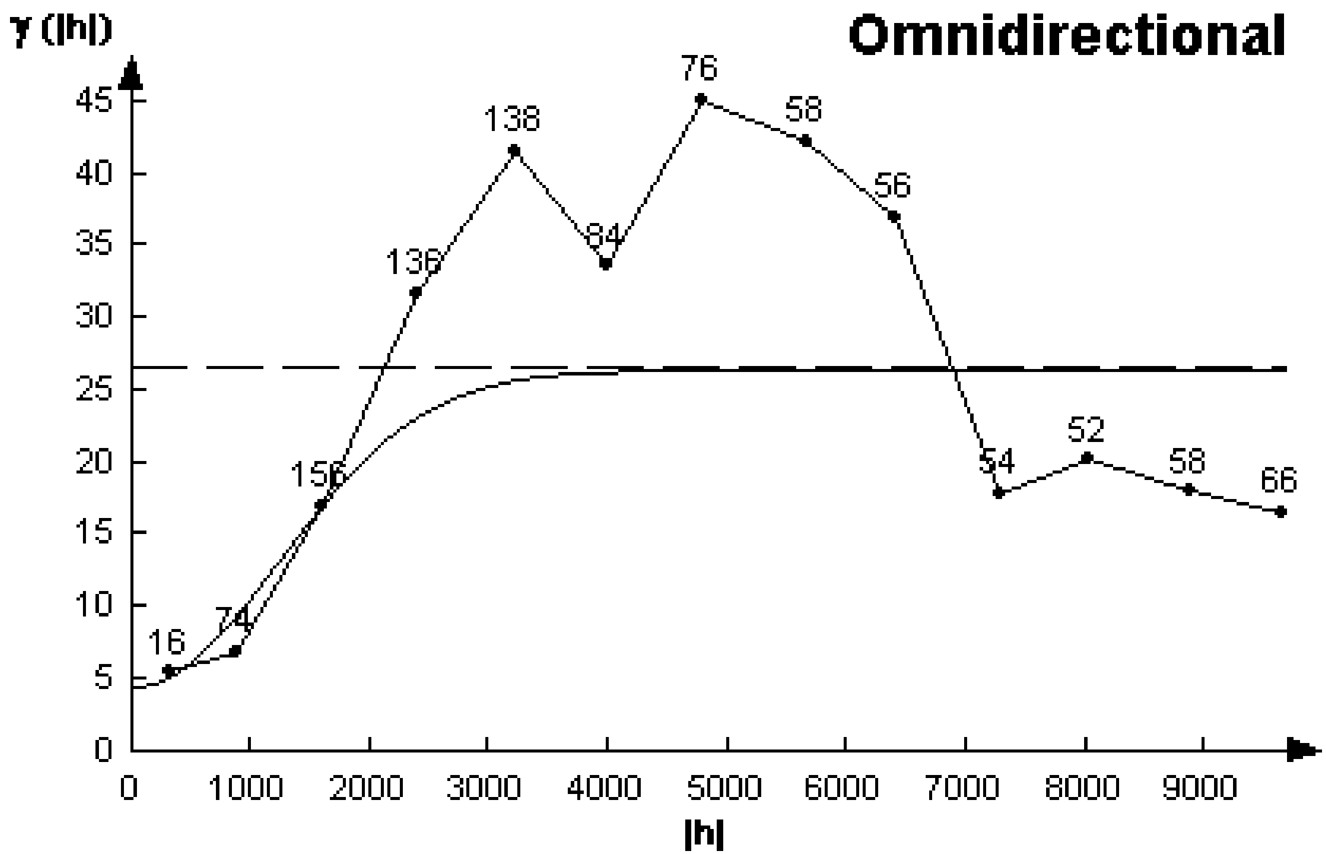
Residual Variograms

Variogram models fitted to residual variograms

Range of spatial correlation for the residuals is about 3000 meters

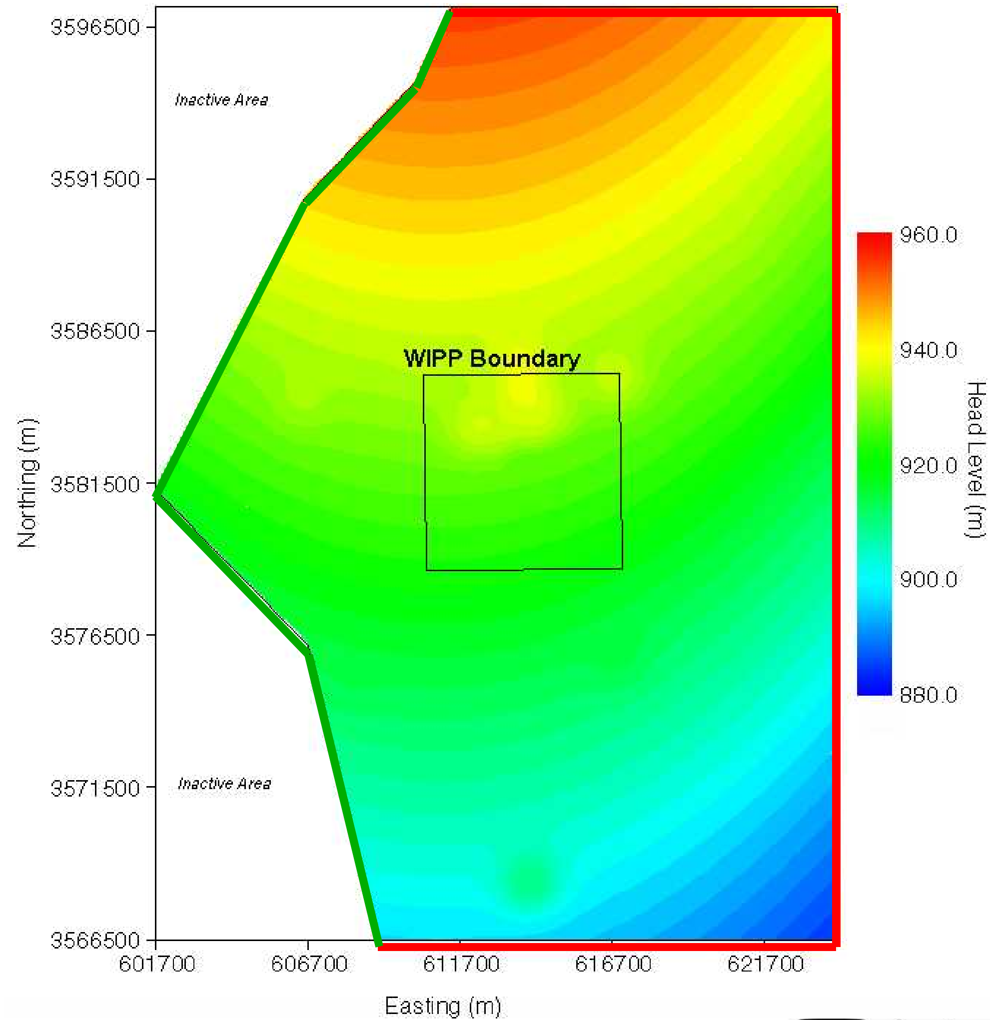


Initial and Boundary Heads

Estimated heads are created as the final result of adding the bivariate Gaussian trend back to the estimated residuals

Fixed Head (red line)

No Flow (green line)

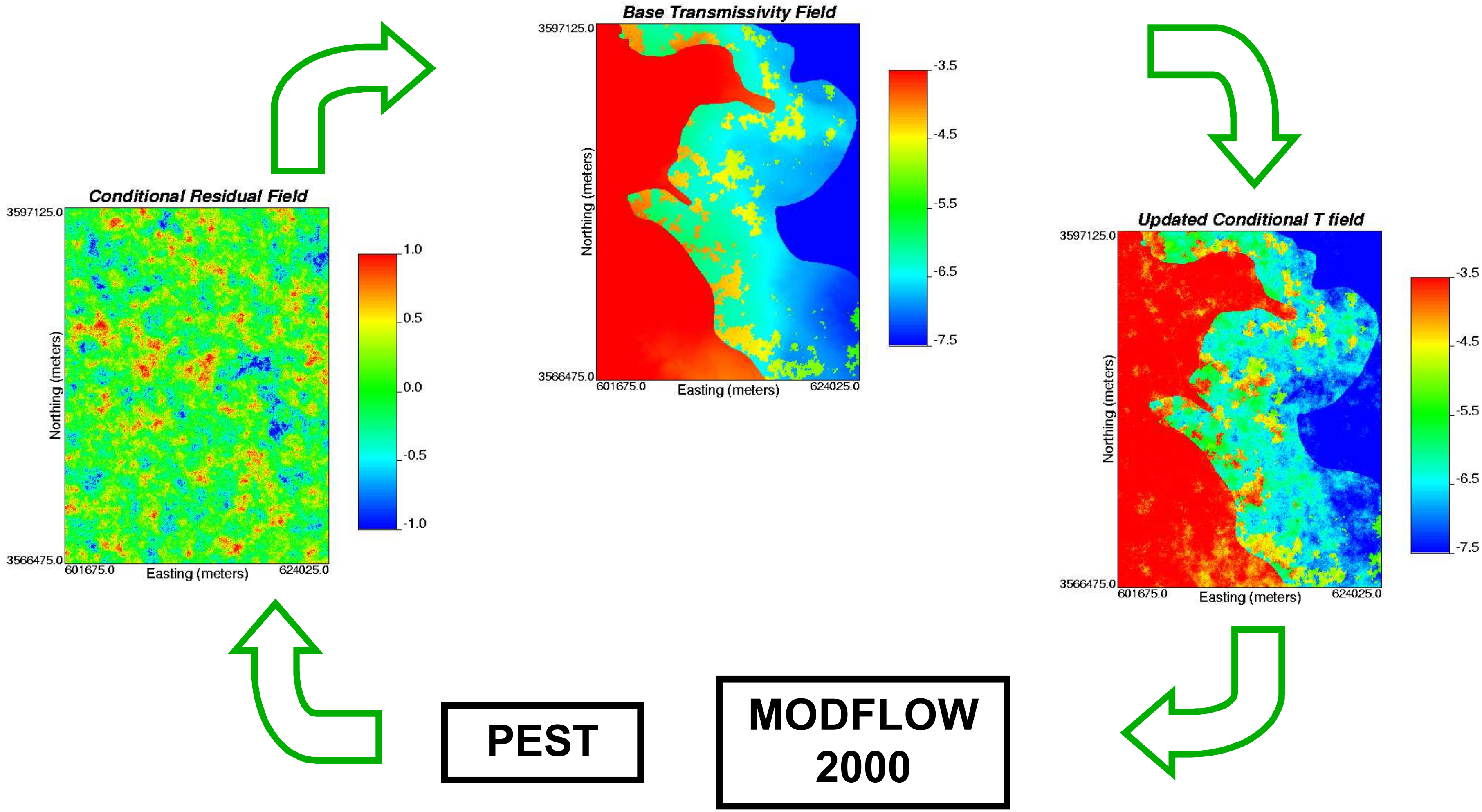


Color scale shows initial heads in meters above sea level

T-Field Calibration Overview

- **Calibration to steady-state and transient heads (drawdown) within model domain**
  - **Steady-state heads collected in 2000**
  - **10 separate pumping tests over 11+ years (October 1985 to December 1996)**
  - **Nearly infinite number of drawdown observations were trimmed to 1332 observations**
    - Resolving response, but computationally tractable
    - 6-104 observations at a single well
    - 64-410 observations for a single test
- **Use MODFLOW 2000 (v. 1.6) with PEST (v. 5.5)**

T-Field Calibration Process

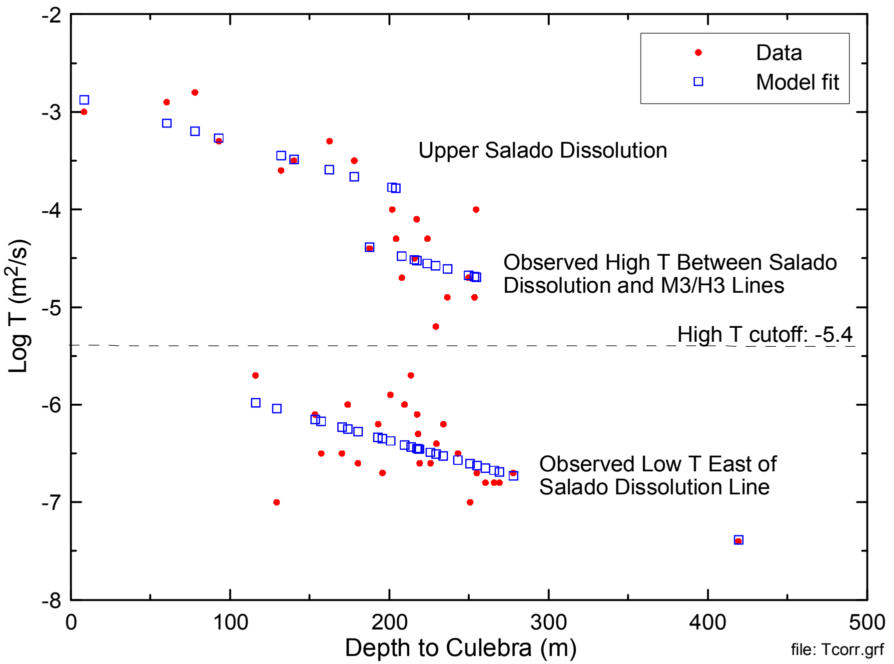


Conditioning to Multiple Data Types

- Base T fields are not conditioned to T measurements
  - They need to honor measured T data
- T fields must reproduce conceptual geologic model
  - Geologic boundaries are crisp; pilot points spread perturbations smoothly
- T fields must be calibrated to measured heads and drawdowns

Base Fields to Seed Fields

Regression models do not honor the measured data ("best fit" line, not a "perfect fit" line)



<u>What does this mean for Culebra modeling?</u>

Need to modify base transmissivity fields to honor the measured T data – use a simulated residual field

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Residual Fields

- **Calculate the residual values between the measured transmissivity and base transmissivity field**
  - **Similar concept to creating initial and boundary head fields**
  - **Calculate residual variogram and use geostatistical simulation to create initial residual fields**
- **Fix the residual values at the measurement points**
- **Use pilot points to update the residual field**

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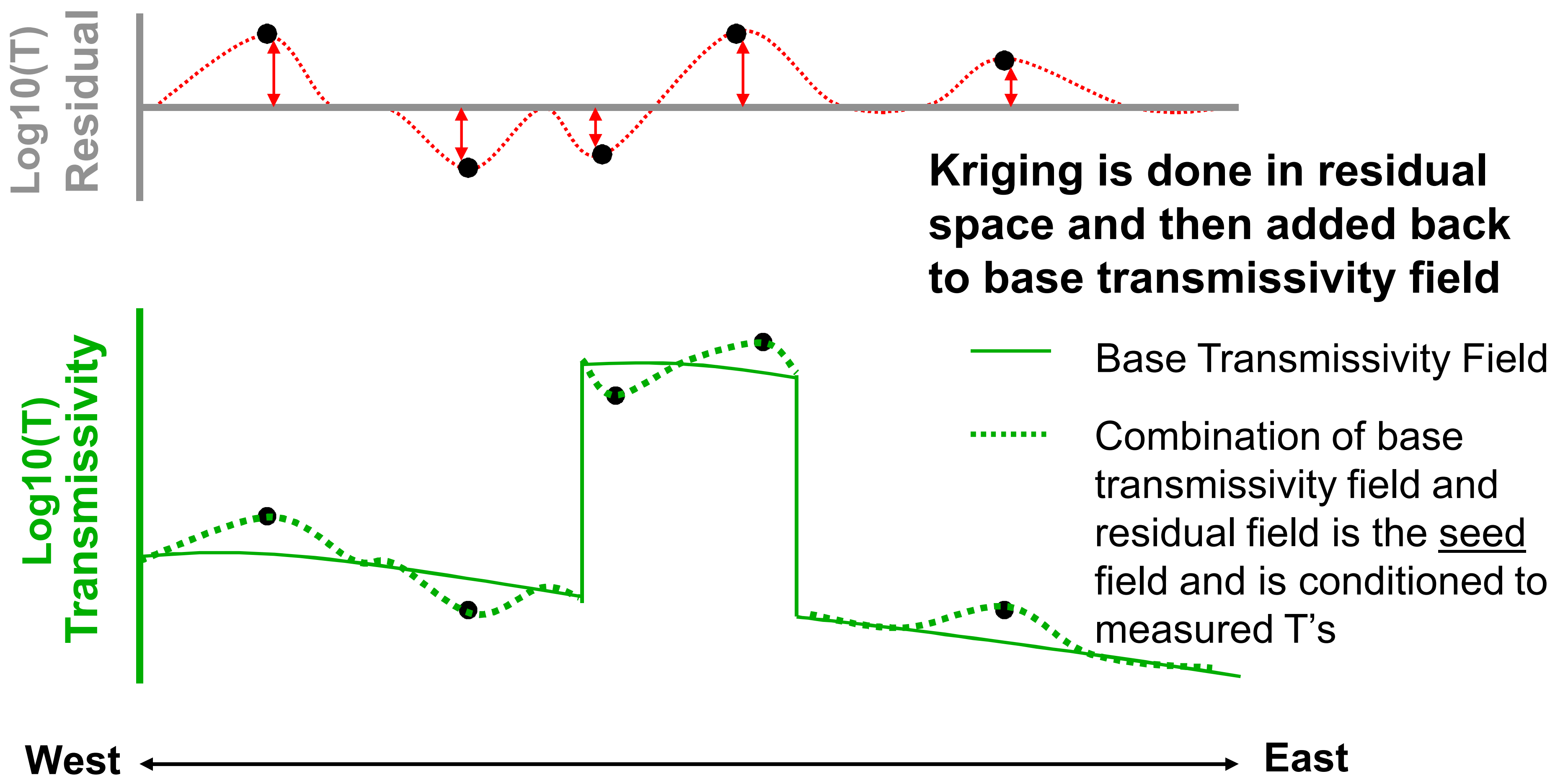
Updating Base T Fields



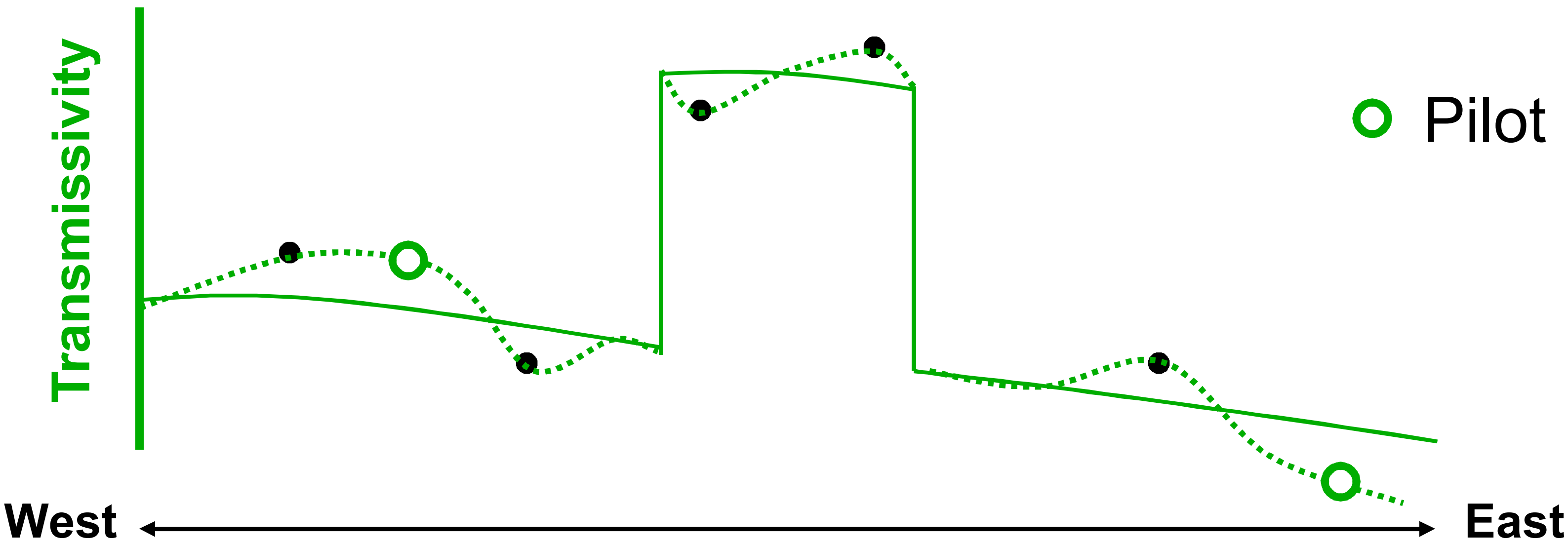
Kriging is done in residual space and then added back to base transmissivity field

Conceptual Cross-Section Through Model Domain

Updating Seed Field

Seed T field honors the measurements at the measurement locations and has a mean equal to that of the base T field, but does not necessarily produce groundwater levels that match observed levels.

Pilot points are used to update the residual field to create a <u>calibrated</u> T field that matches the observed heads



Conceptual Cross-Section Through Model Domain

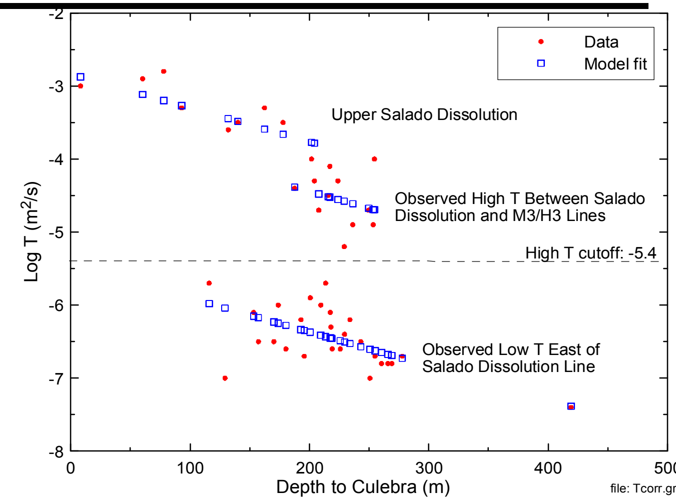
Maintain Geologic Model

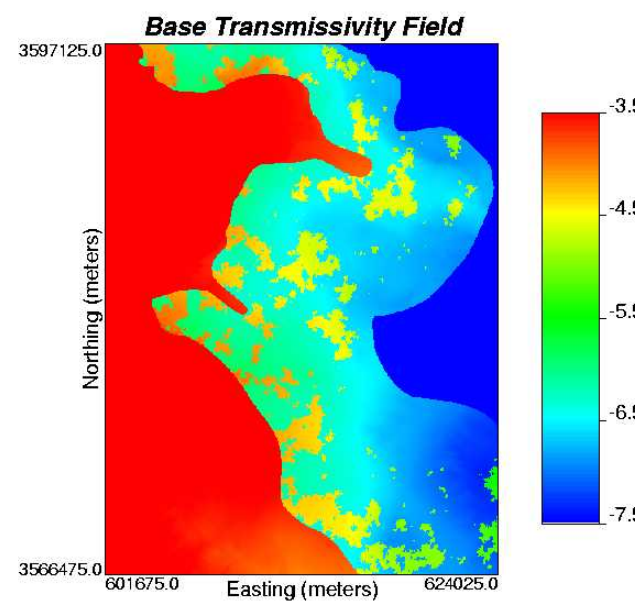
High T zones in base fields are created stochastically, independently of head data

Calibration to heads must be able to overturn stochastic classification (H to L; L to H)

Pilot points in center of domain, are constrained to +/- 3 orders of magnitude in residual space

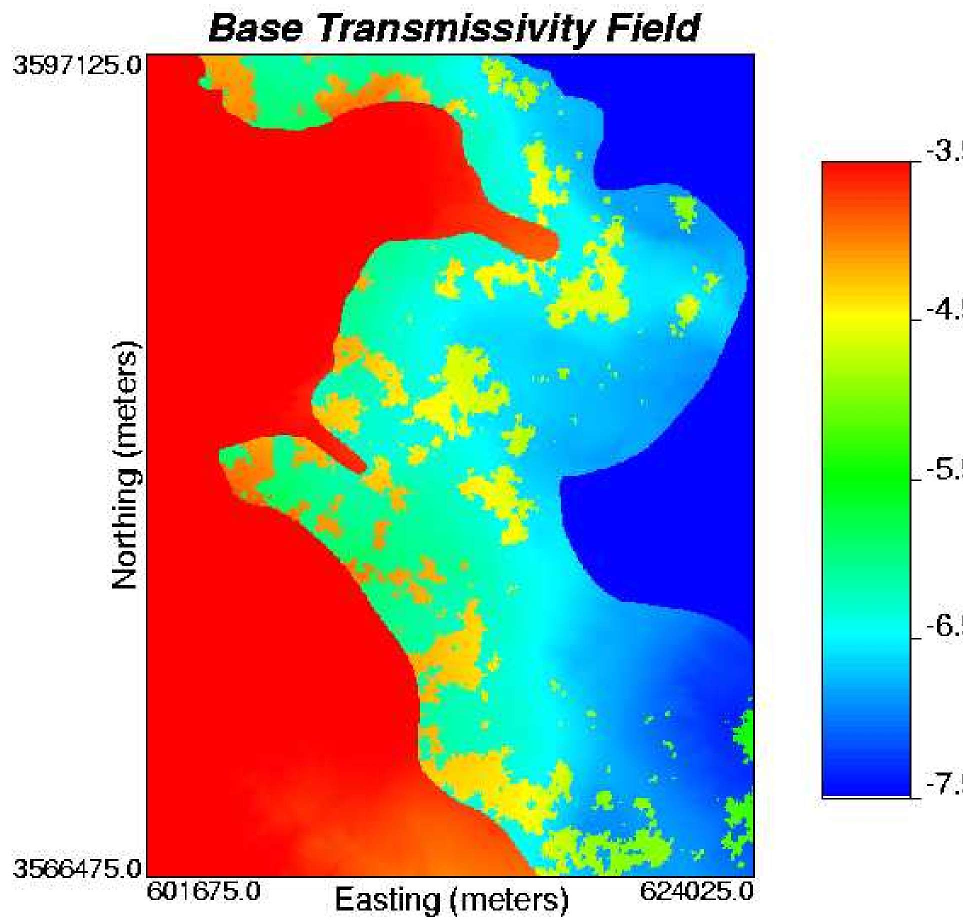
In low and high T zones, limit is +/- order of magnitude





Maintain Geologic Model (Cont.)

- Sharp zone boundaries in conceptual model are maintained during calibration
- Calibration influence of any pilot point, and regularization calculations, are limited to zone in which that pilot point is located
- Three geologic zones in model control how head/drawdown data can modify T



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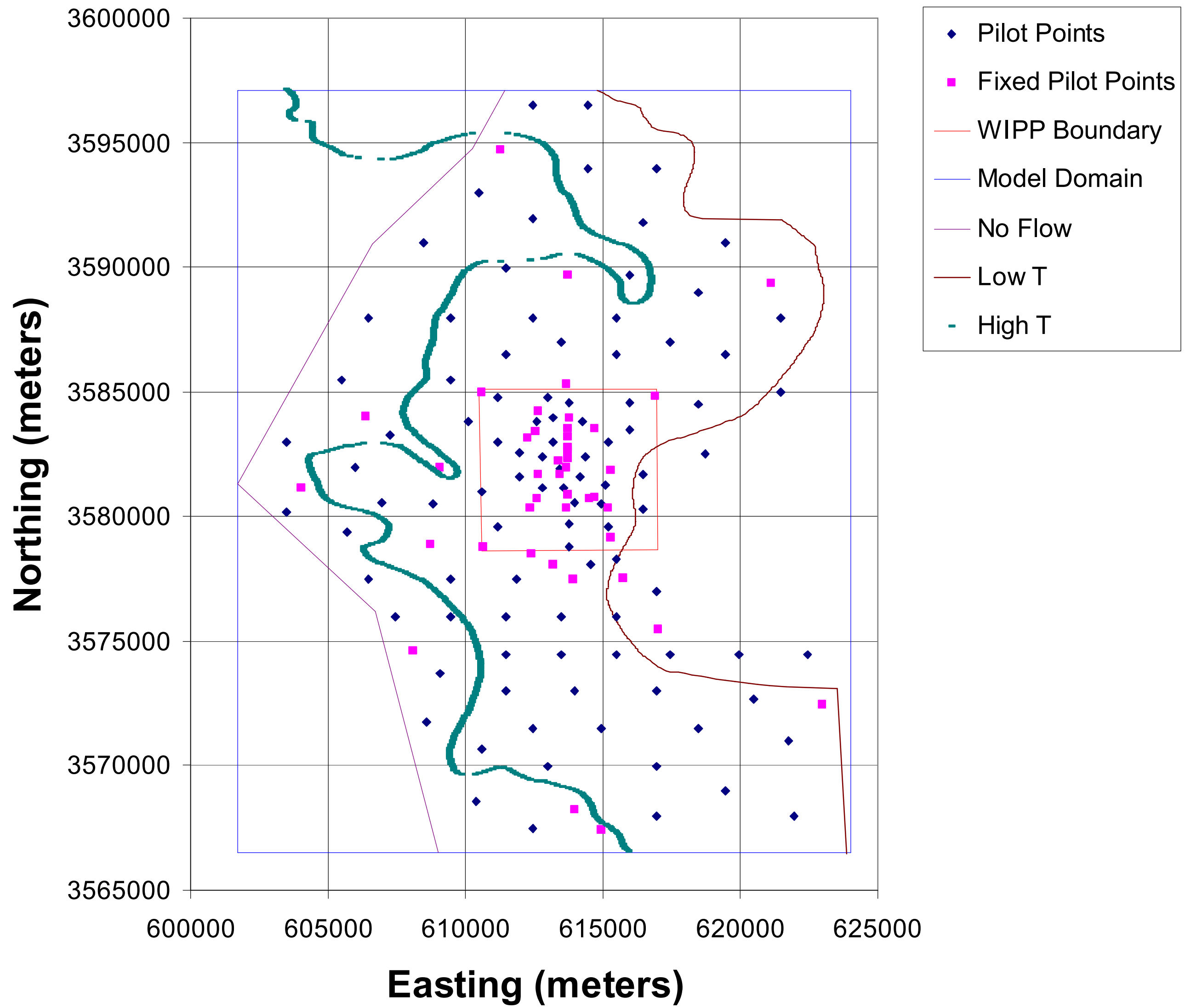
Pilot Points

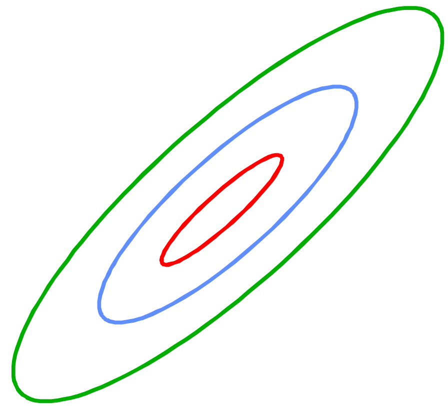
Total of 99 adjustable pilot points

Locations are on a semi-regular grid that is adjusted to account for specific pumping – observation well combinations



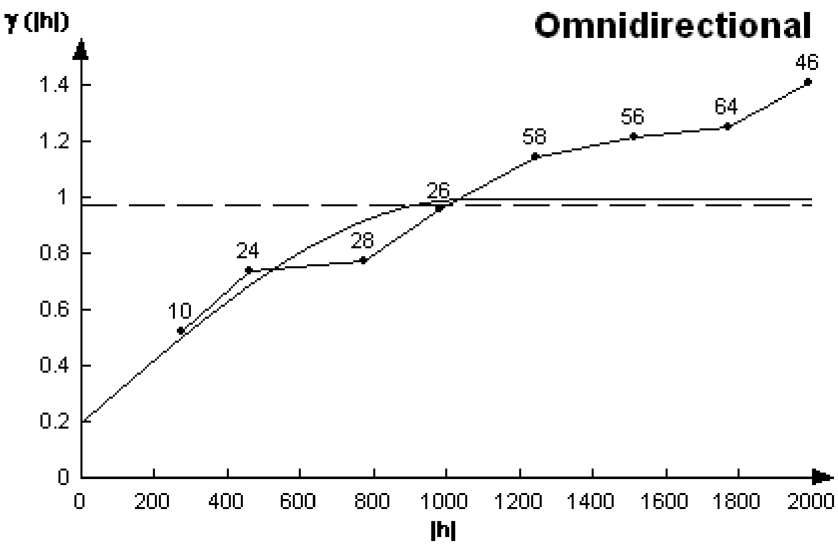
Pilot Points (Cont.)

- **Choose locations in the model domain and update their properties to produce better fit to measured heads ("calibration points")**
- **Spread influence of each point to neighboring model cells by using the spatial covariance function as a weighting scheme**



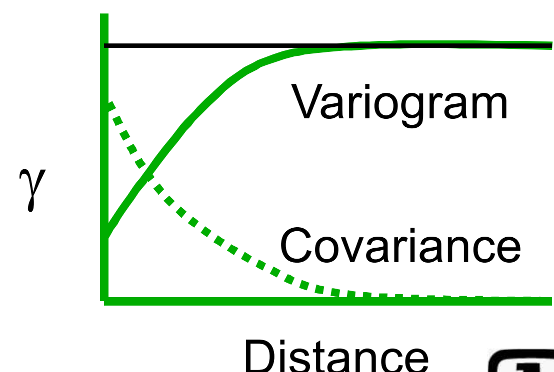
Pilot Points (Cont.)

The variogram calculated on the residuals between the base transmissivity field and the measured transmissivities (46 points) provides the pilot point weight as a function of distance



Variogram of base and measured transmissivity residuals

The actual weight is the covariance value that is the complement of the variogram



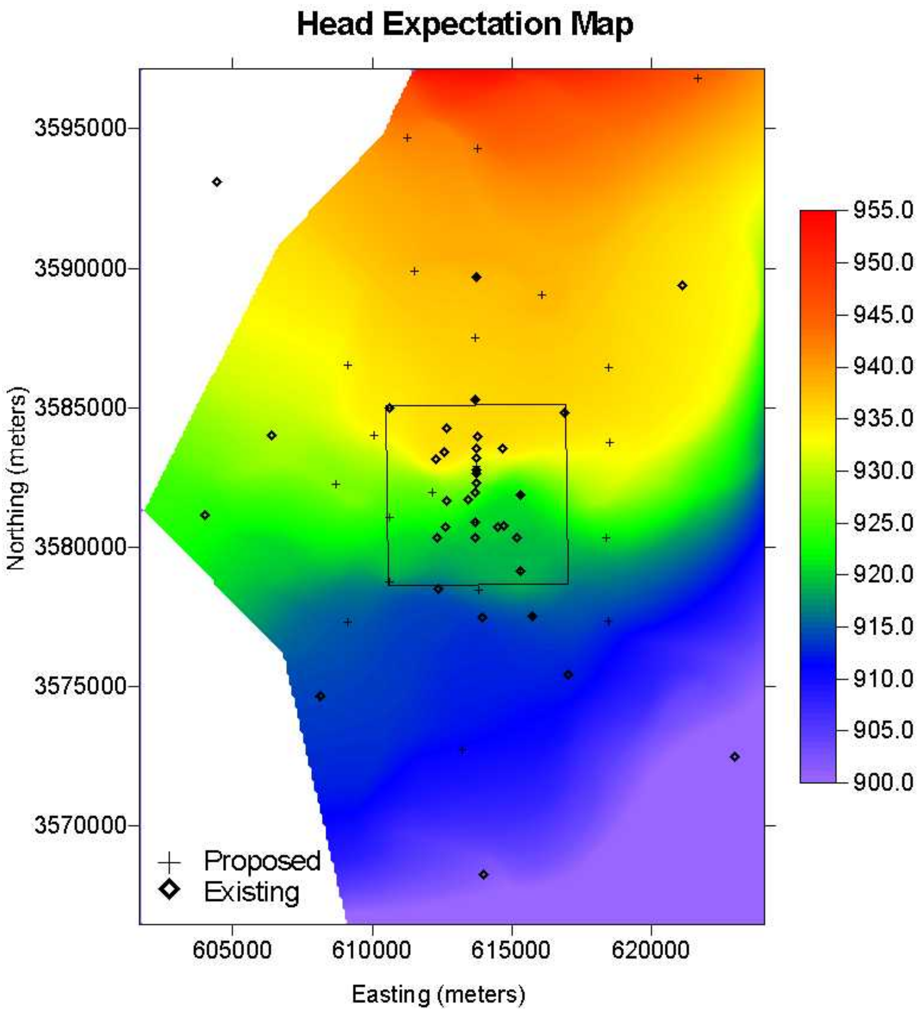
Objective Function

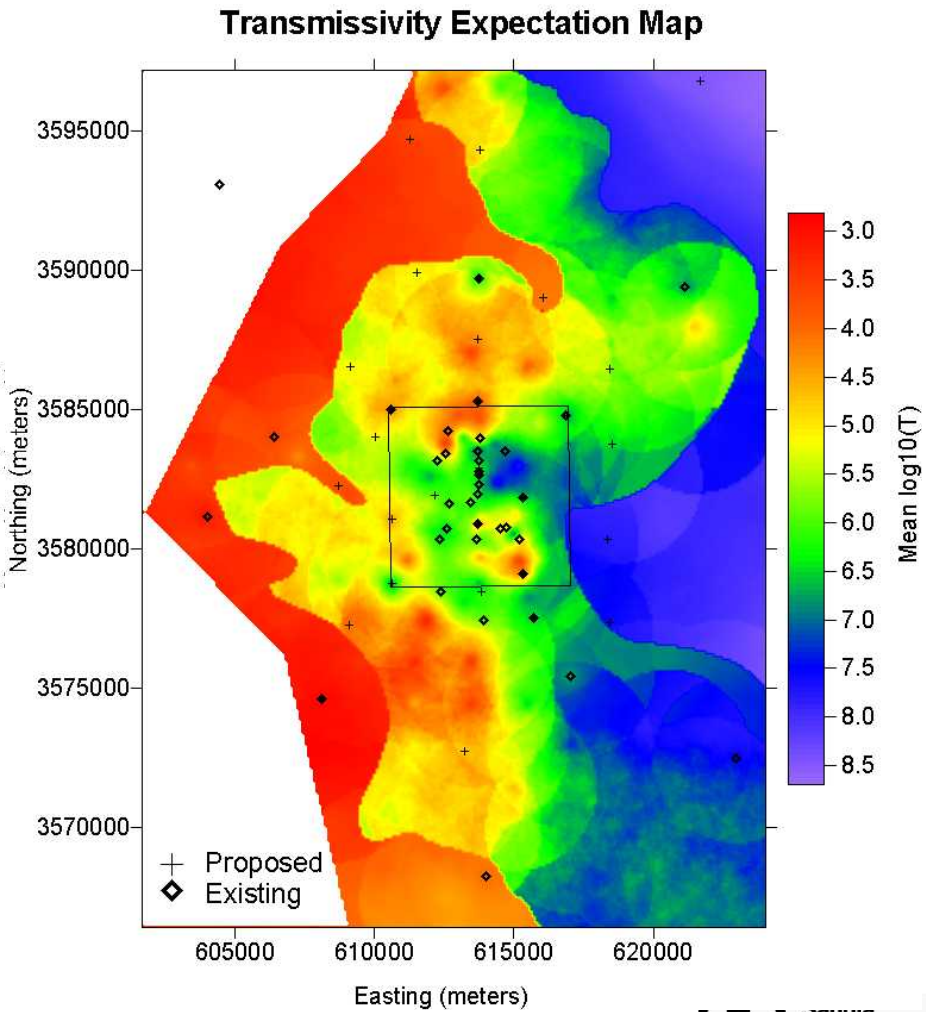
- **The objective function has two components:**
  - **1) Minimize weighted SSE between measured and modeled heads**
  - **2) Minimize weighted SSE between pilot points (maximally smooth T field)**

$$\phi = \sum_{i=1}^{N_H^{obs}} W_i^{obs} (H_i^{obs} - H_i^{calc})^2 + \sum_{j=1}^{N_{PP}} \sum_{k=j}^{N_{PP}} W_{jk}^{reg} (PP_j - PP_k)^2$$

Second component of the objective function is the regularization piece and is necessary to make the solution numerically stable (decreases the effective number of pilot points)

Calibration Results: Head and T





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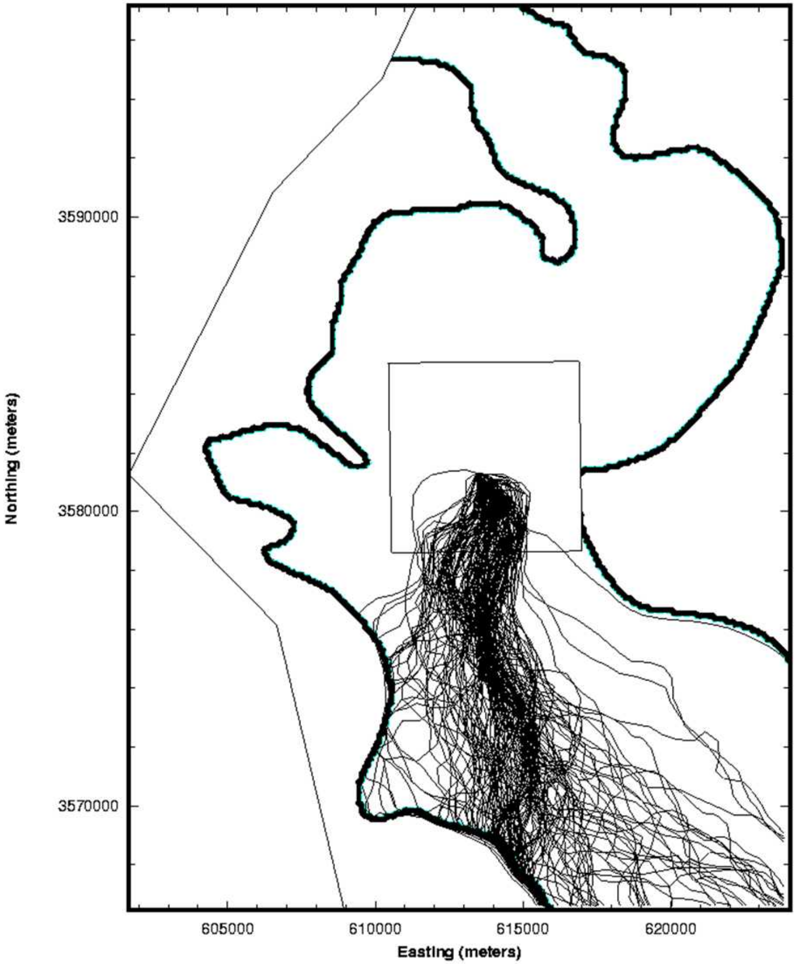
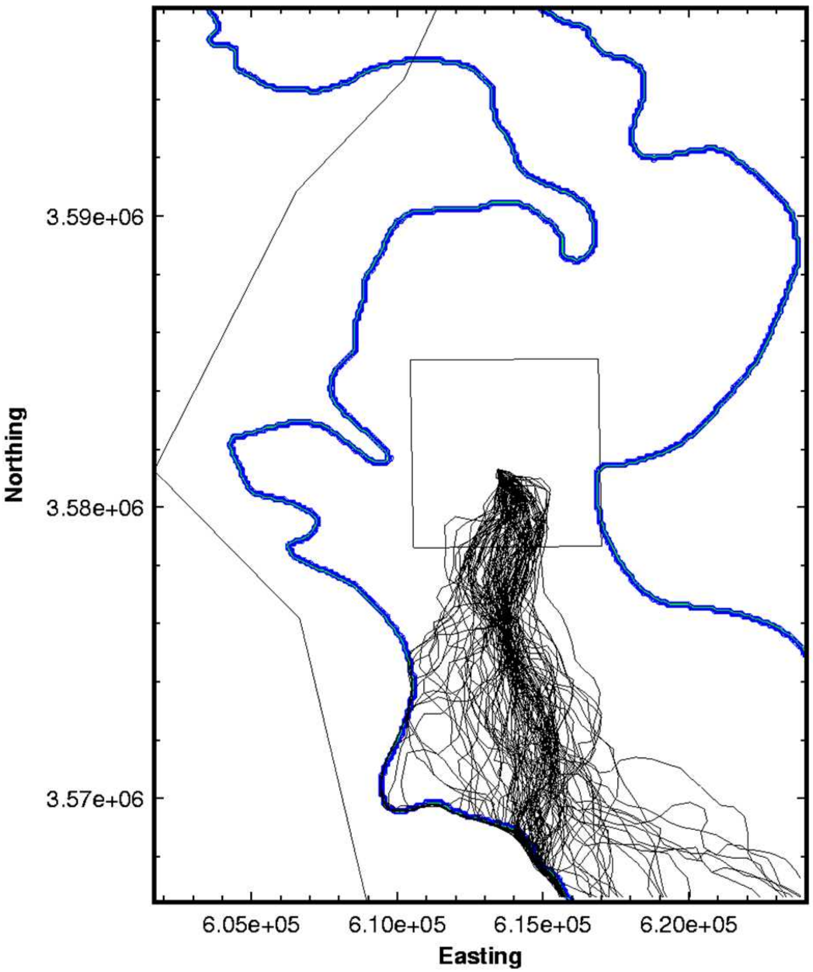
Particle Tracks

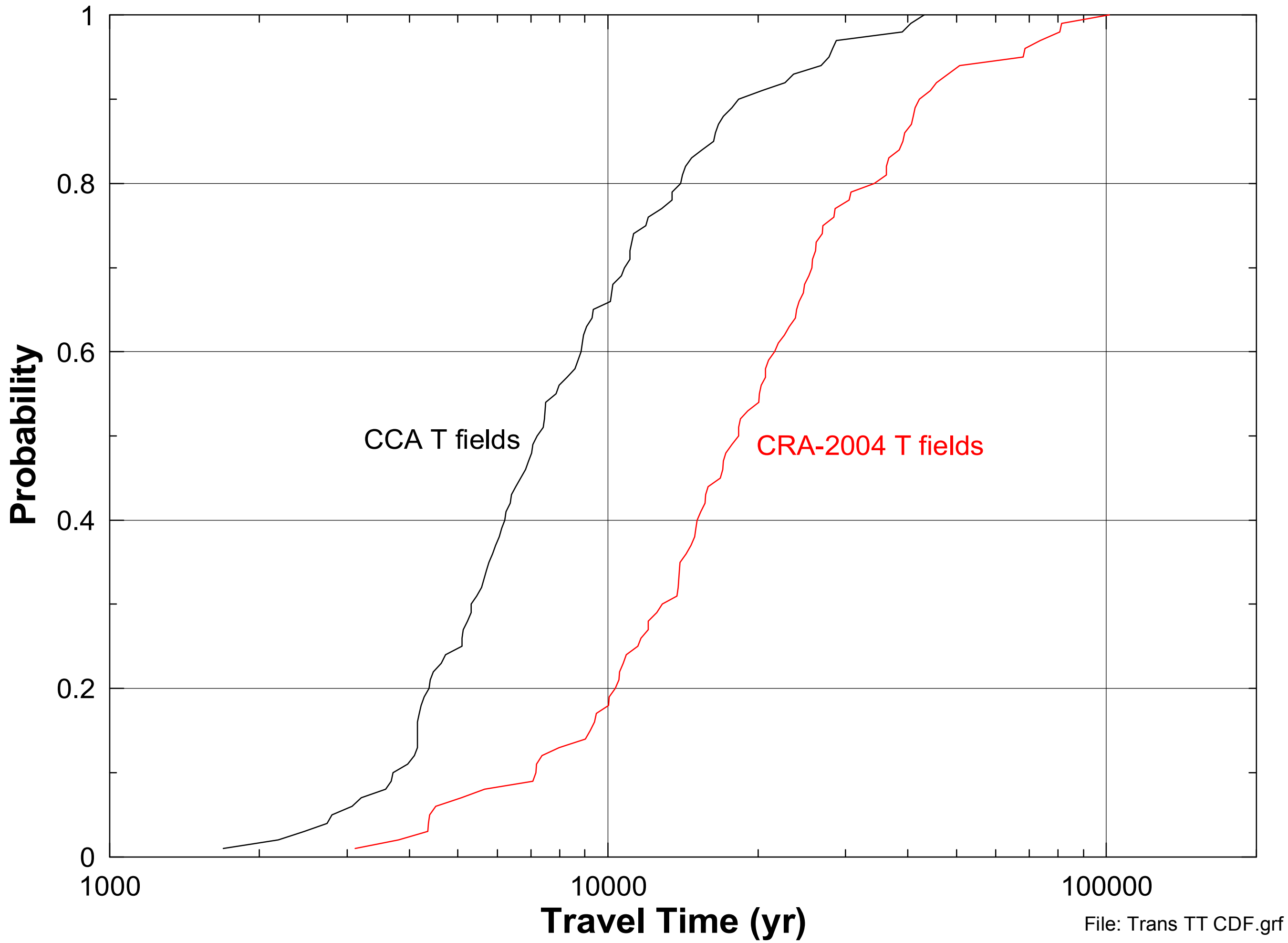
All Calibrated Fields



100 Accepted Fields

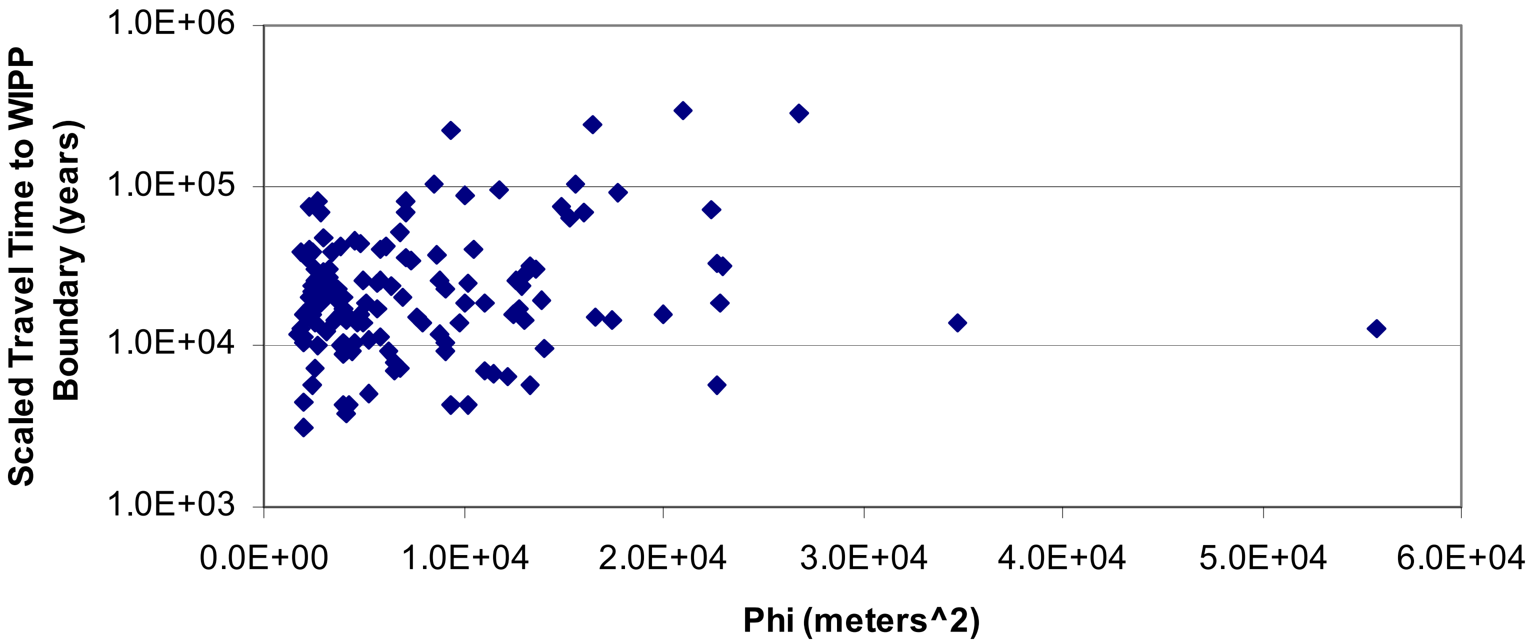


Travel Times



Travel Time vs. Calibration

No relationship between level of calibration and travel time



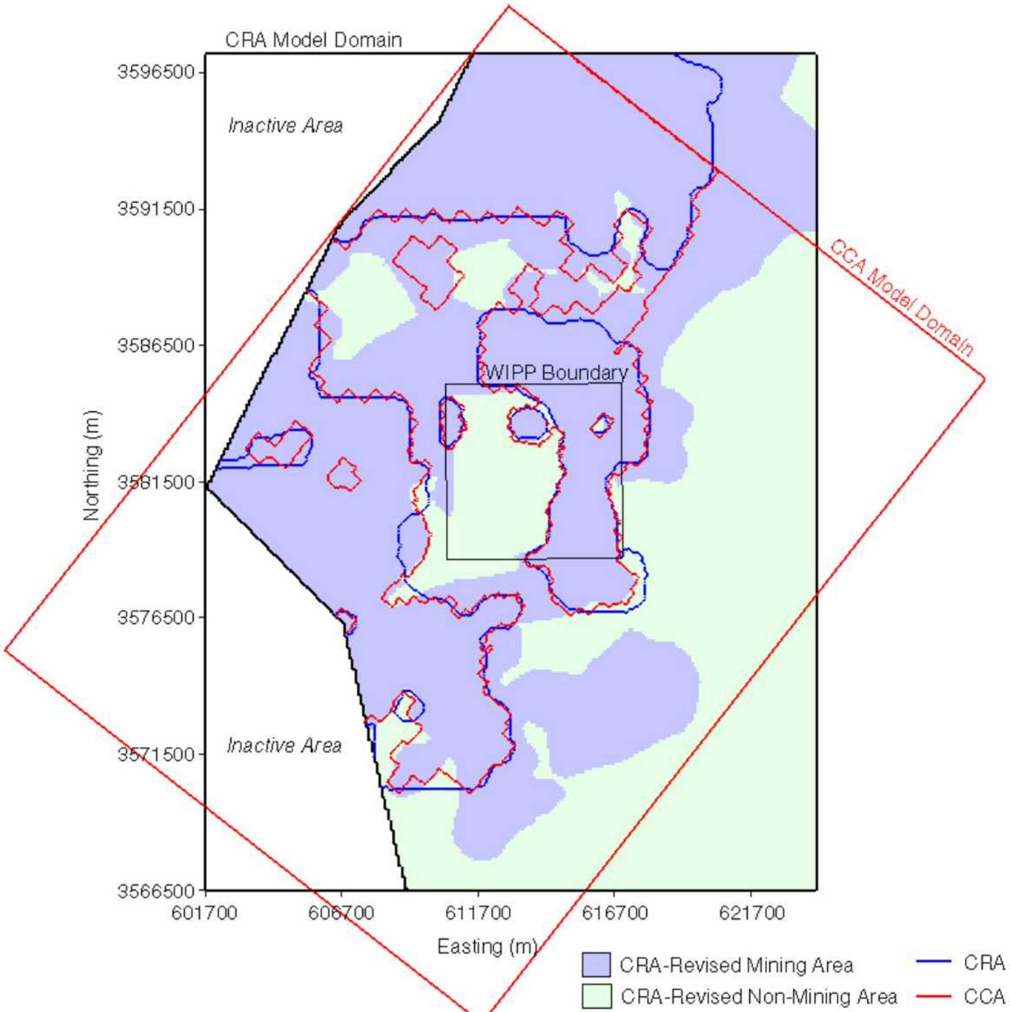
Phi is weighted SSE and includes regularization component

Mining Modifications

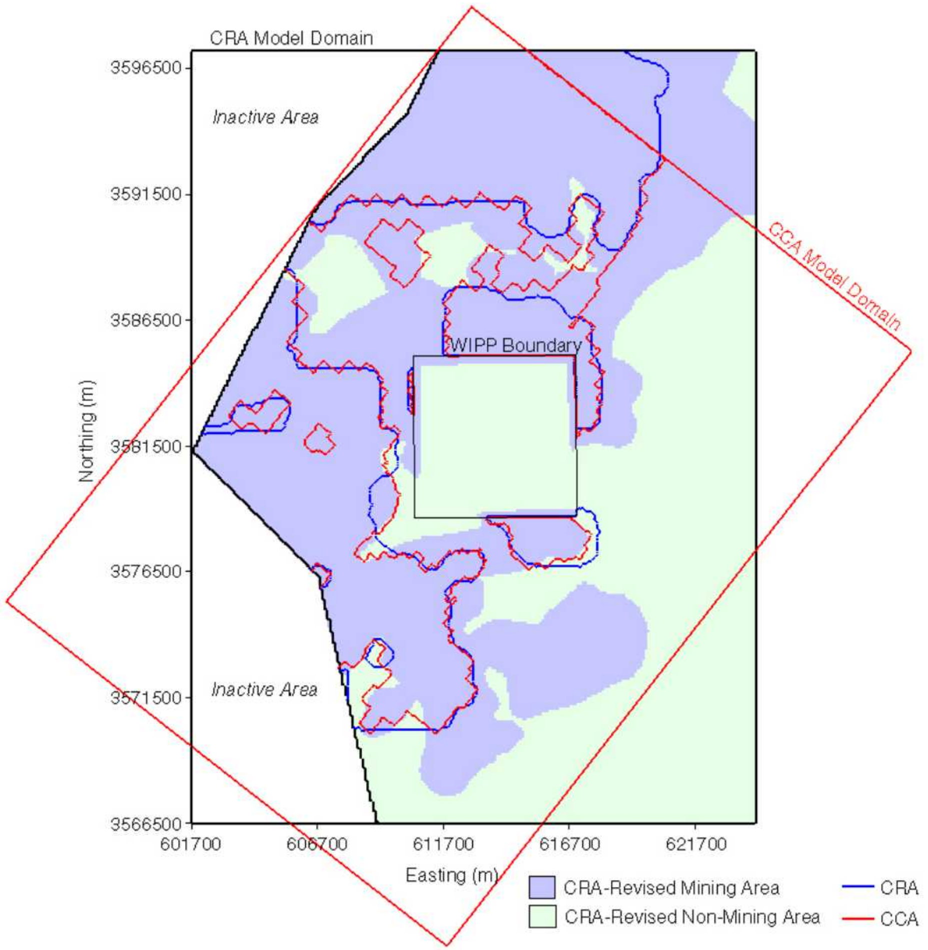
Mining Modification Overview

- Obtain the sampled values for the random mining modification factor (100 vectors x 3 replicates).
- Map potential areas of future potash mining onto the groundwater modeling domain for both full and partial mining scenarios.
- Apply the mining modification factor to the 100 stochastically calibrated T-fields. This will produce 600 mining-modified T-fields (100 vectors x 2 mining scenarios x 3 replicates).

Full Mining Map



Partial Mining Map



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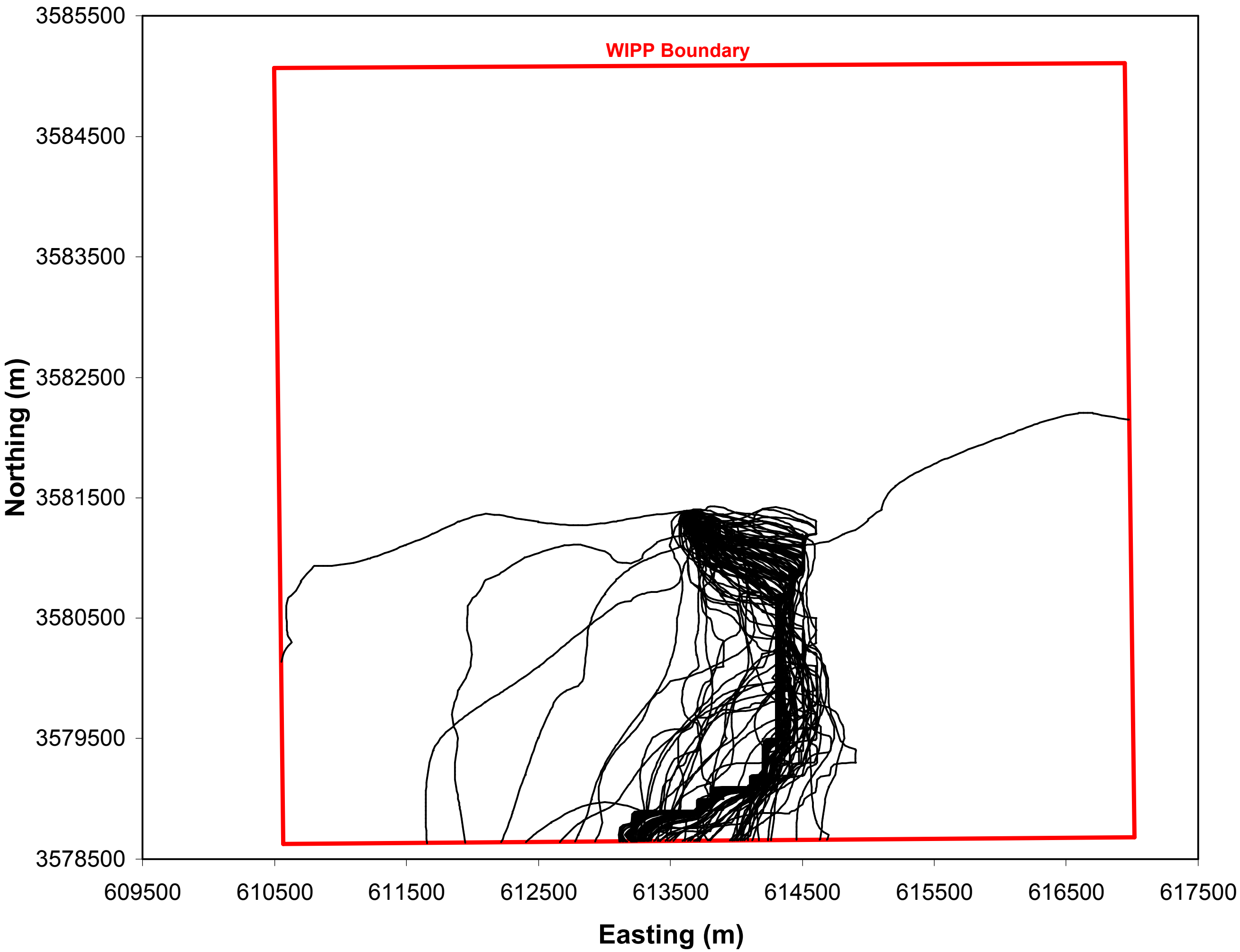
Flow Calculations

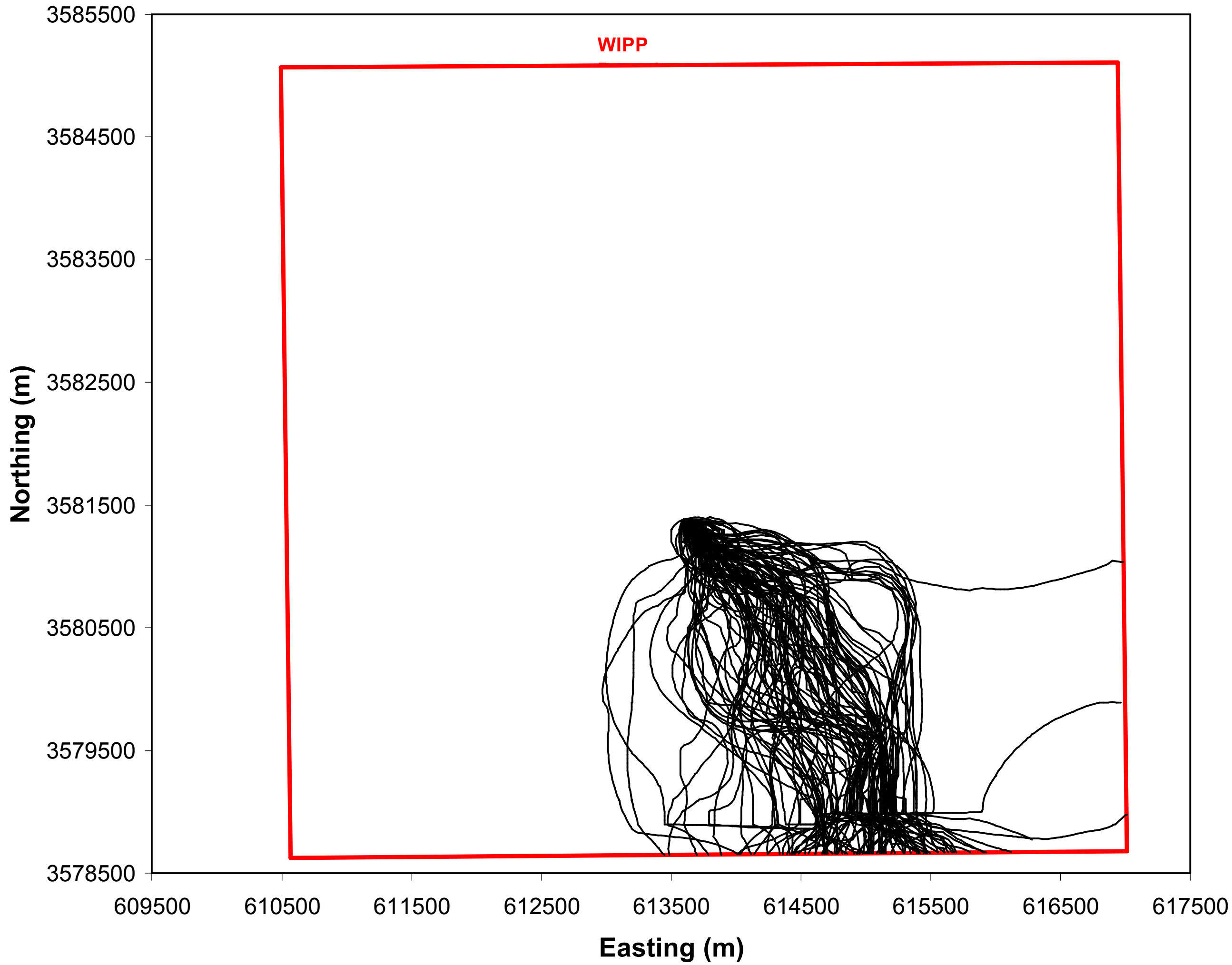
Flow Calculation Overview

- **Perform steady-state flow simulations for each mining-modified T-field using MODFLOW 2000 (MF2K).**
- **Perform particle tracking using the new mining-affected flow-fields to determine travel times to the LWB.**
- **Refine the flow field to smaller grid size for use in the radionuclide transport calculations.**

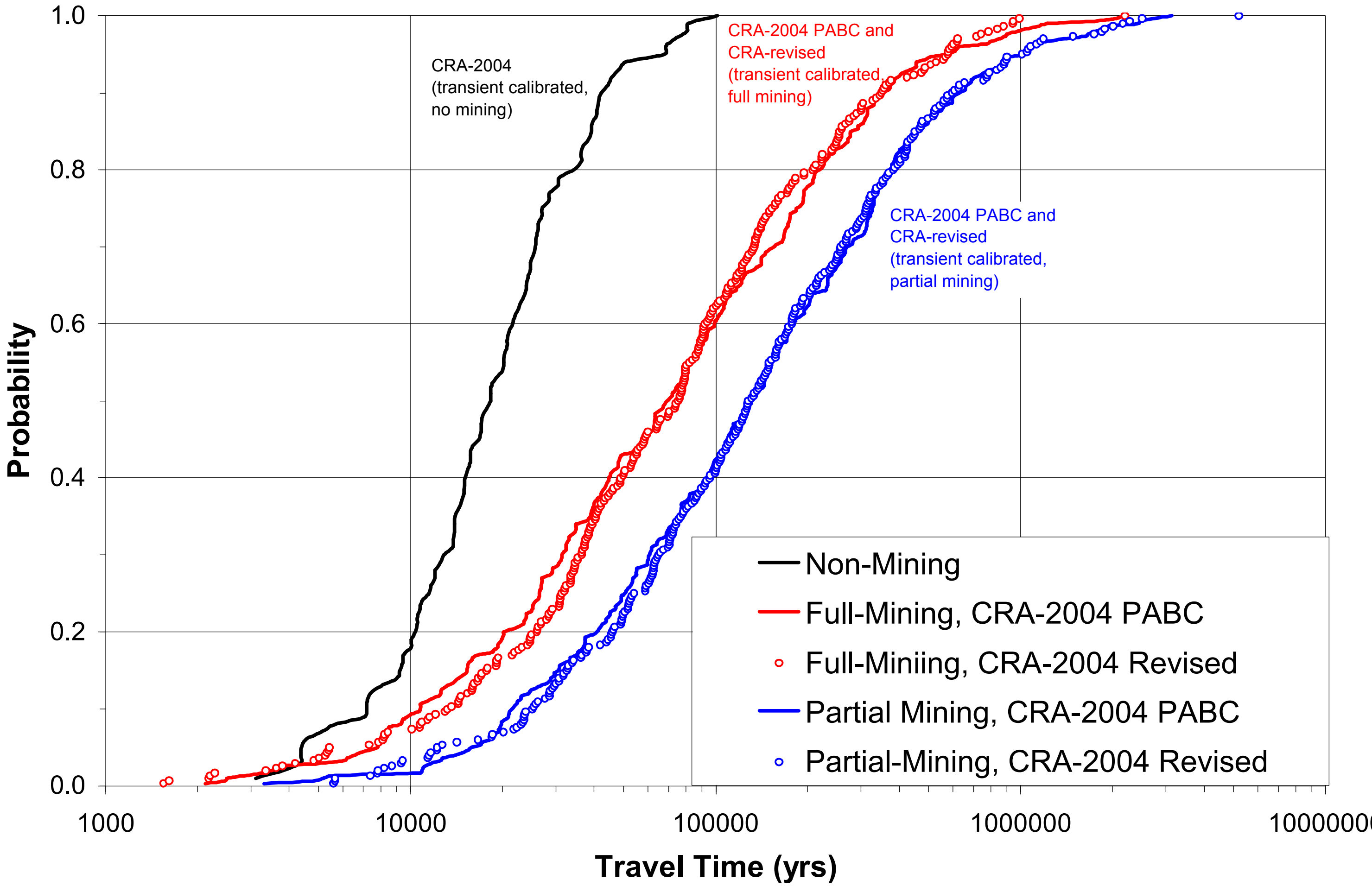
Particle Tracking (R1, Full Mining)



Particle Tracking (R1, Partial Mining)



Advective Travel Times



Transport Calculations

Transport Simulations

- **Calculate transport of 241Am,239Pu, 230Th, 234U**
- **Am present as Am(III)**
- **Pu present as PU(III) or PU(IV)**
- **Th present as Th(IV)**
- **U 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

Deterministic Transport Parameters

Parameter	Units	Value
Longitudinal Dispersivity	m	0
Transverse Dispersivity	m	0
Fracture Tortuosity	-	1
Diffusive Tortuosity	-	.11
Material Grain Density	kg/m^3	2.82e+3
^{241}Am Half-life	s	1.364e+10
Am^{3+} Diffusion Coefficient	m^2/s	3.0e-10
^{239}Pu Half-life	s	7.594e+11
Pu^{3+} Diffusion Coefficient	m^2/s	3.0e-10
Pu^{4+} Diffusion Coefficient	m^2/s	1.53e-10
^{230}Th Half-life	s	2.43e+12
Th^{4+} Diffusion Coefficient	m^2/s	1.53e-10
^{234}U Half-life	s	7.716e+12
U^{4+} Diffusion Coefficient	m^2/s	1.53e-10
U^{6+} Diffusion Coefficient	m^2/s	4.26e-10

Uncertain Transport Parameters

Parameter	Units	Distribution	Range	Median
Advective Porosity	-	Log uniform	[1.0e-04, 1.0e-2]	1.00e-03
Matrix Porosity	-	Cumulative	[1.0e-01, 2.5e-01]	1.60e-01
Matrix Half-block Length	m	Uniform	[5.0e-02, 5.0e-01]	2.75e-01
Oxidation State Index	-	Uniform	[0.0, 1.0]	5.00e-01
Climate Index	-	Cumulative	[1.0, 2.25]	1.17e+00
Am^{3+} Matrix K_d	m^3/kg	Log uniform	[2.0e-02, 4.0e-01]	9.00e-02
Pu^{3+} Matrix K_d	m^3/kg	Log uniform	[2.0e-02, 4.0e-01]	9.00e-02
Pu^{4+} Matrix K_d	m^3/kg	Log uniform	[7.0e-01, 1.0e+1]	2.60e+00
Th^{4+} Matrix K_d	m^3/kg	Log uniform	[7.0e-01, 1.0e+1]	2.60e+00
U^{4+} Matrix K_d	m^3/kg	Log uniform	[7.0e-01, 1.0e+1]	2.60e+00
U^{6+} Matrix K_d	m^3/kg	Log uniform	[3.0e-05, 2.0e-02]	7.70e-04

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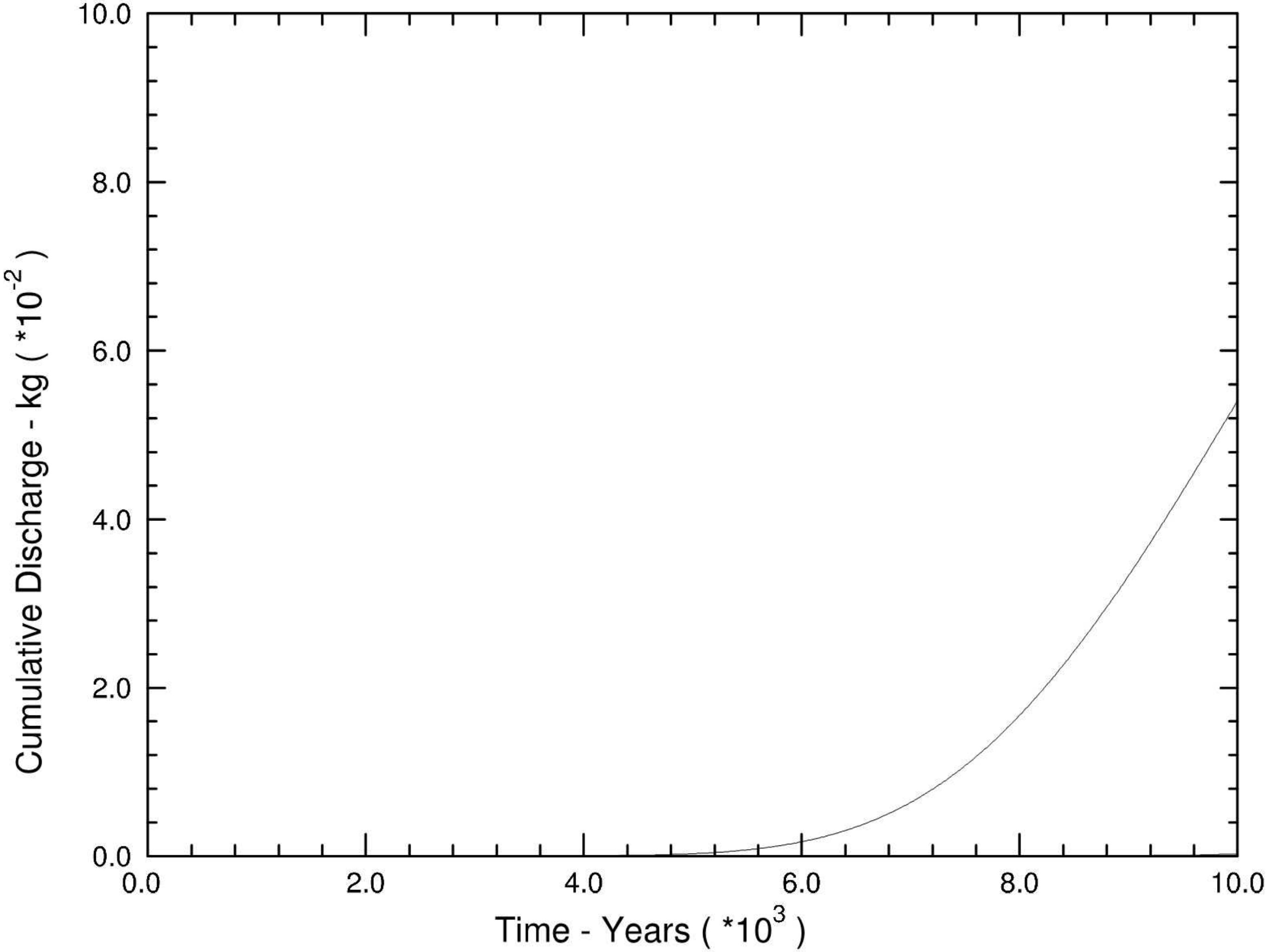
Sampling

- 600 velocity fields (100 T-fields x 2 mining scenarios x 3 replicates)
- Uncertain geochemical and transport parameters selected using Latin Hypercube Sampling (100 vectors x 3 replicates)
- Each parameter vector matched with a partial mining and full mining velocity field
- Total of 600 transport simulations

SNL WIPP CRA1A: CULEBRA RADIONUCLIDE TRANSPORT (SECOTP2D)

U234 Cumulative Discharge at LWB, Partial Mining, R1



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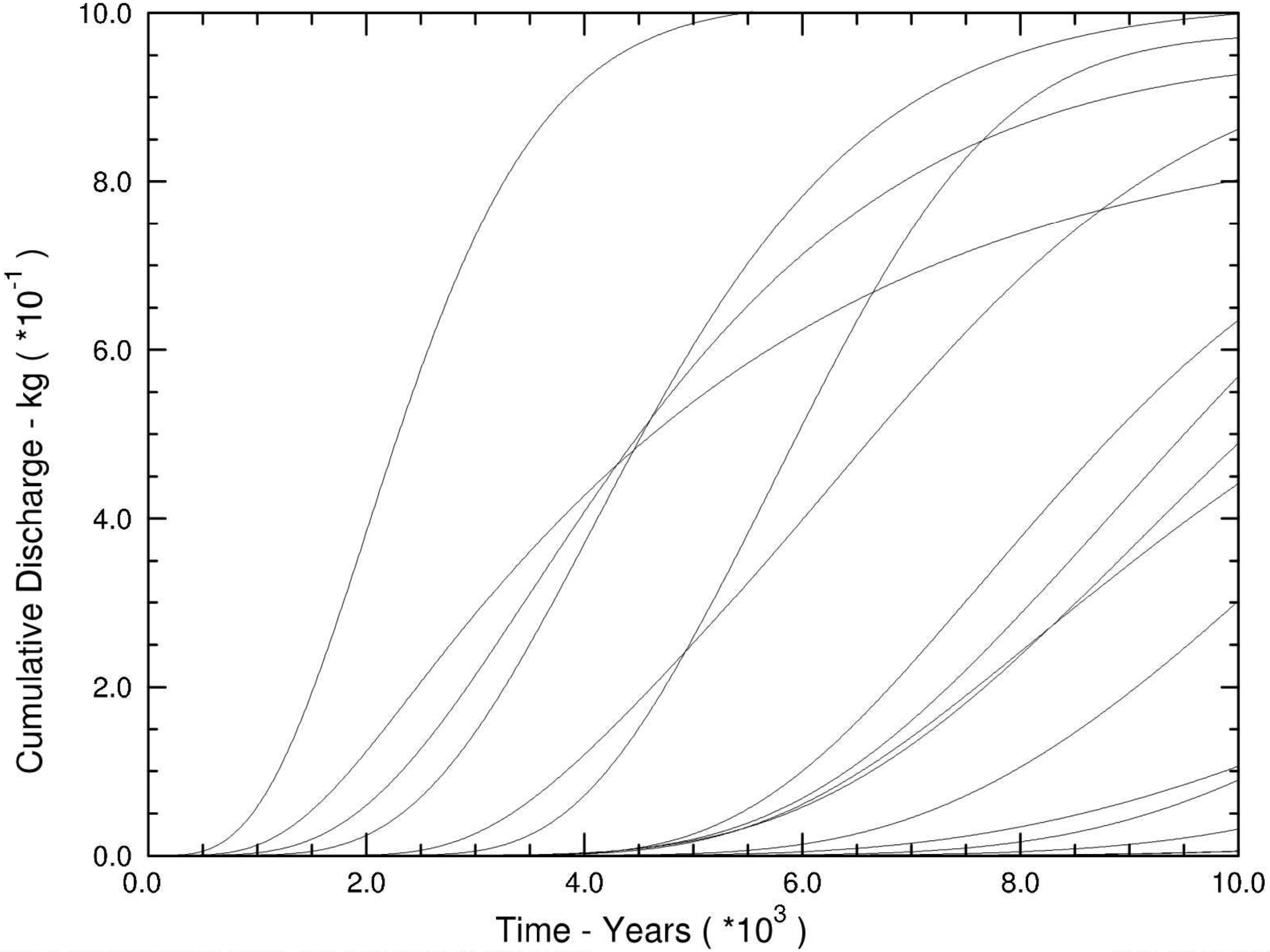
SPLAT_PA96_2 1.02 12/15/03

SNL WIPP CRA1A: CULEBRA RADIONUCLIDE TRANSPORT (SECOTP2D)

U234 Cumulative Discharge at WPA, Partial Mining, R1



PAWORK:[SHARED.JFKANNE.WRK.V05.SPLAT]SPLAT_ST2D_CRA1A_R1_PM_U234_MT1_SP.INP;5

SPLAT_PA96_2 1.02 12/08/03 11:59:12

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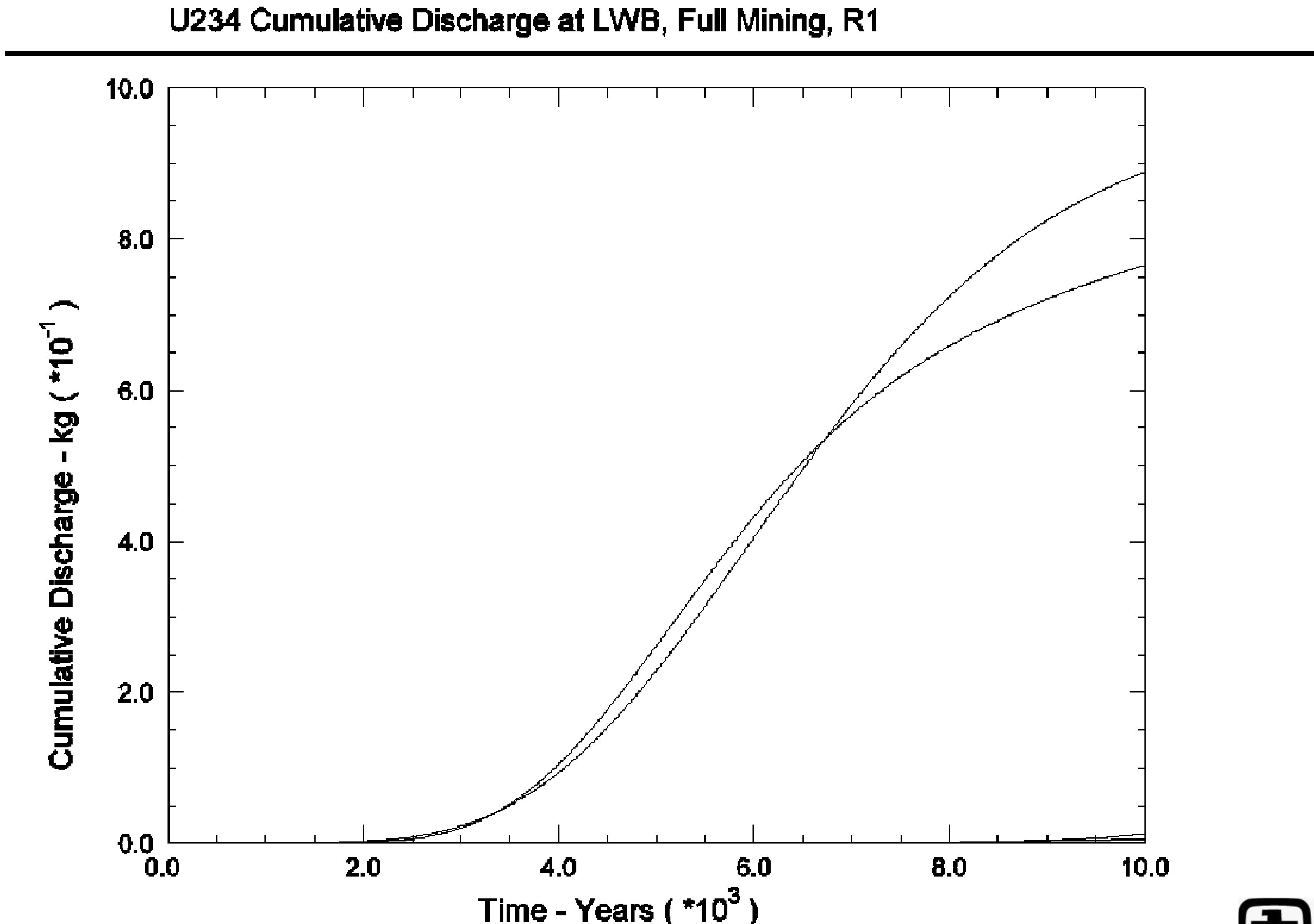
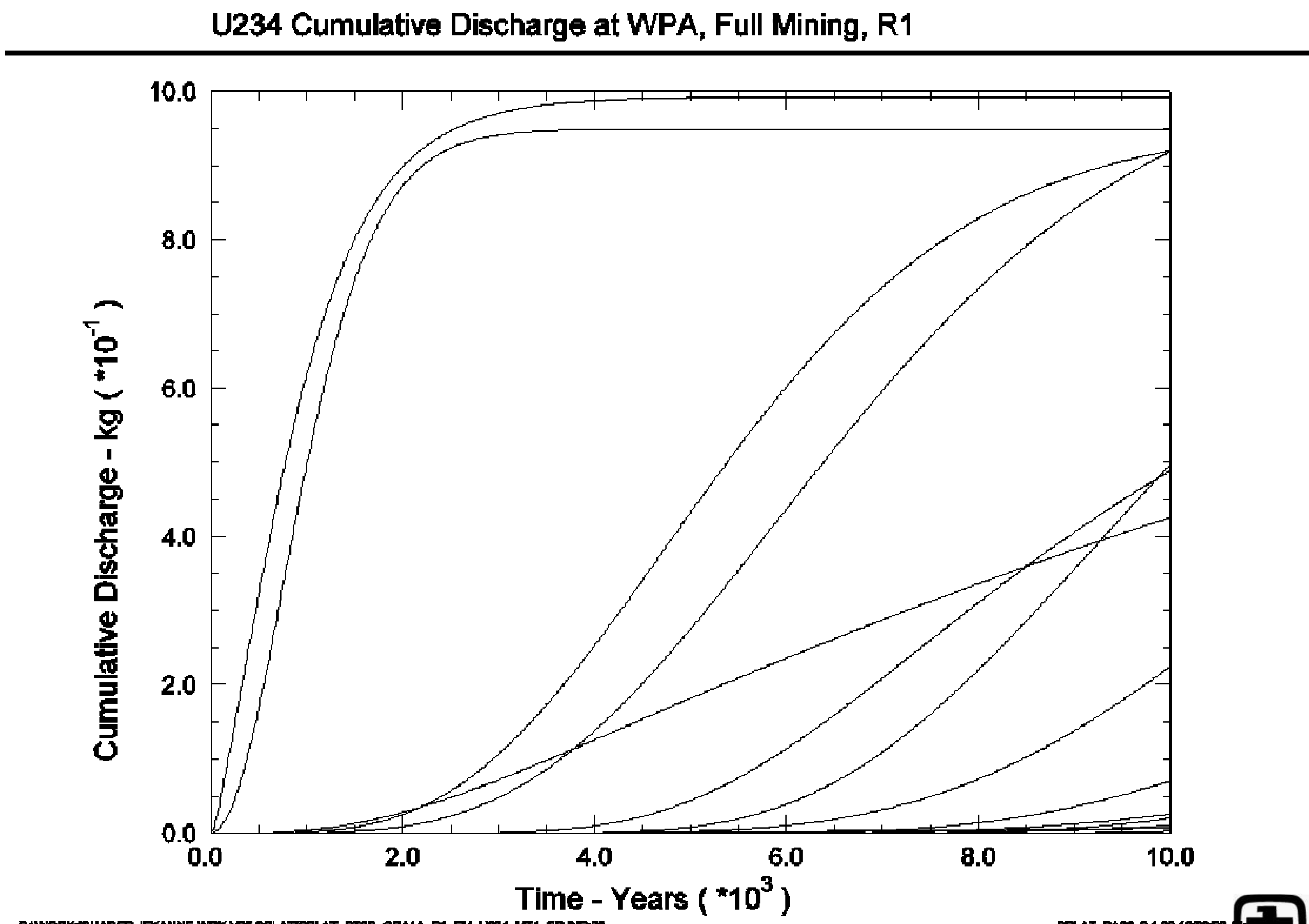
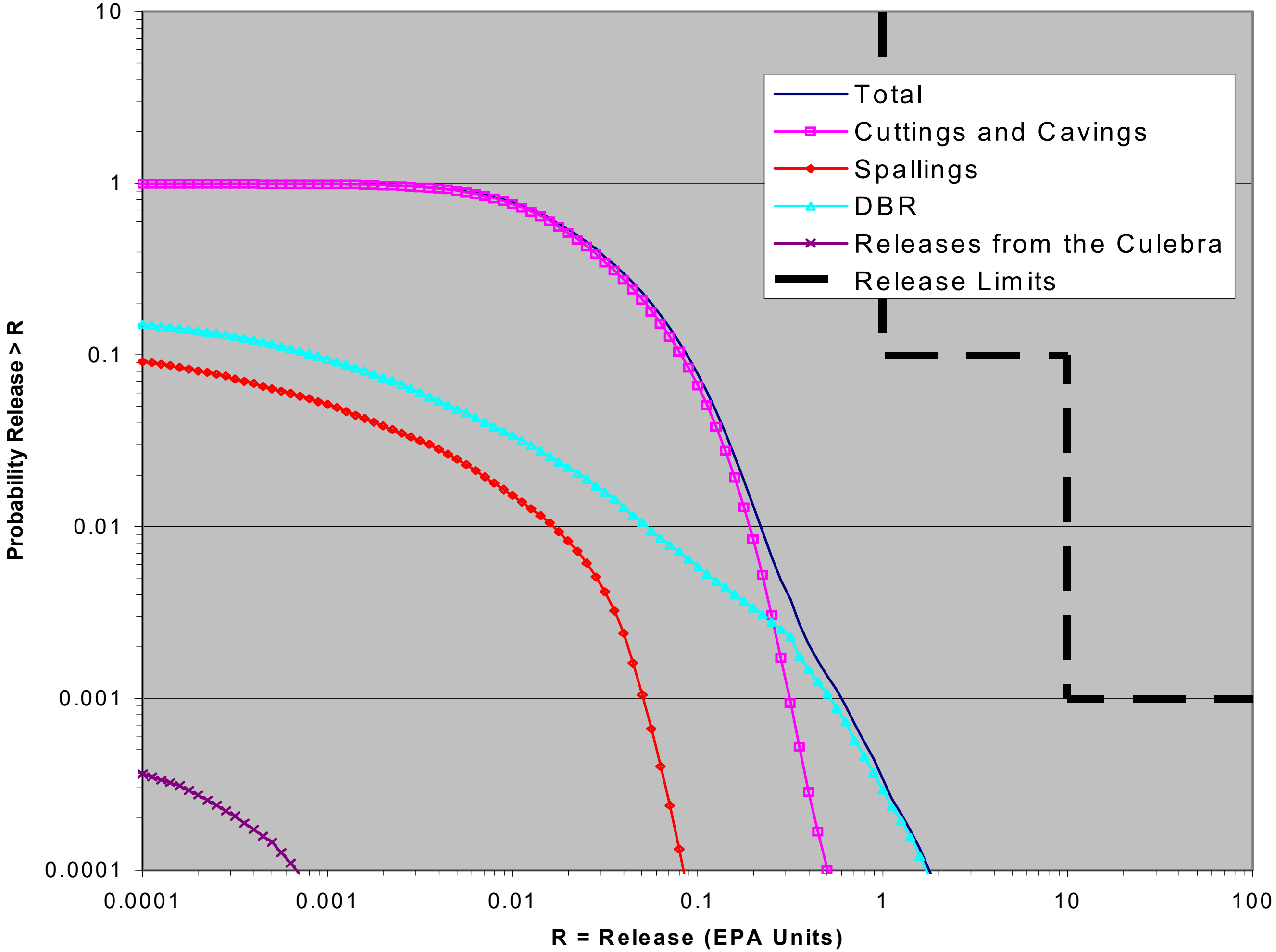

U234 Cumulative Discharge at LWB, Full Mining, R1
Cumulative Discharge - kg (*10^-1)
Time - Years (*10^3)
0.0
2.0
4.0
6.0
8.0
10.0


U234 Cumulative Discharge at WPA, Full Mining, R1
Cumulative Discharge - kg (*10^-1)
Time - Years (*10^3)
0.0
2.0
4.0
6.0
8.0
10.0

Culebra Releases Compared to Other Mechanisms (PABC)



Transport Conclusions

- **Only ^{234}U transported to LWB in considerable amounts in 10,000 years**
- **When convolved with probabilistic models for drilling intrusion, Salado flow and transport, and fluid movement up borehole, the probability of significant release from Culebra is negligible.**
- **Releases to LWB not large enough for meaningful sensitivity analysis**
- **Transport of ^{234}U past WPA boundary is sensitive to oxidation state.**
- **K_d for U(VI) is lower than for U(IV), resulting in faster transport.**