UNRAVELING COMPLEXITY THROUGH FATE AND TRANSPORT NUMERICAL SIMULATIONS IN A TIDALLY-INFLUENCED, HETEROGENOUS, MULTI-SYSTEM, DENSITY DRIVEN REGIME

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ACKNOWLEDGEMENTS

1. Jack Button – Parsons PM
2. Jeff Snell – Parsons PG

Source: just cute animals

AGENDA

1. Groundwater Modeling
2. Site example – why is this presentation relevant?
3. Site Setting
4. Geological / hydrogeological Environment
5. Groundwater model workflow
6. Calibration
7. Results and conclusions

The Ground Water Modeling Process

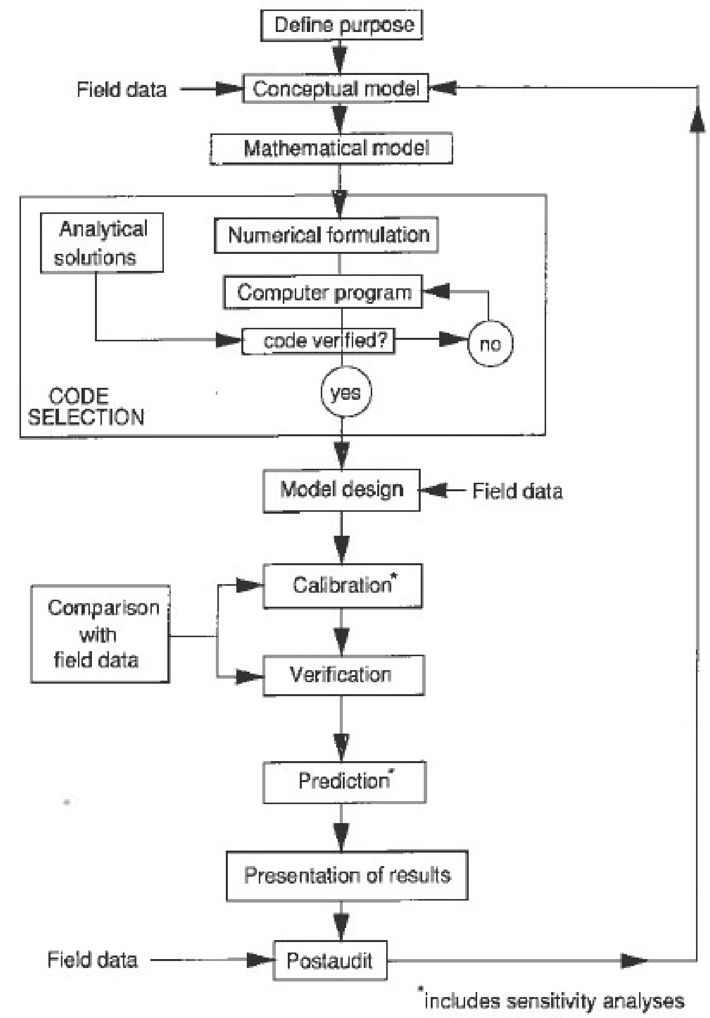


Fig. 1.1 Steps in a protocol for model application.

Analytical versus Numerical

Analytical

- F(x) = x – 15
  - Solution: add both sides by 15 then: x=15
  - Conceptually simple (sort of)
  - Theoretically based
  - Exact solution
  - Time consuming in multivariate equations

Solving groundwater flow analytically

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

where

K_{xx}, K_{yy}, and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (L/T);

h is the potentiometric head (L);

W is a volumetric flux per unit volume representing sources and/or sinks of water, with W<0.0 for flow out of the ground-water system, and W>0.0 for flow into the system (T^{-1});

S_S is the specific storage of the porous material (L^{-1}); and

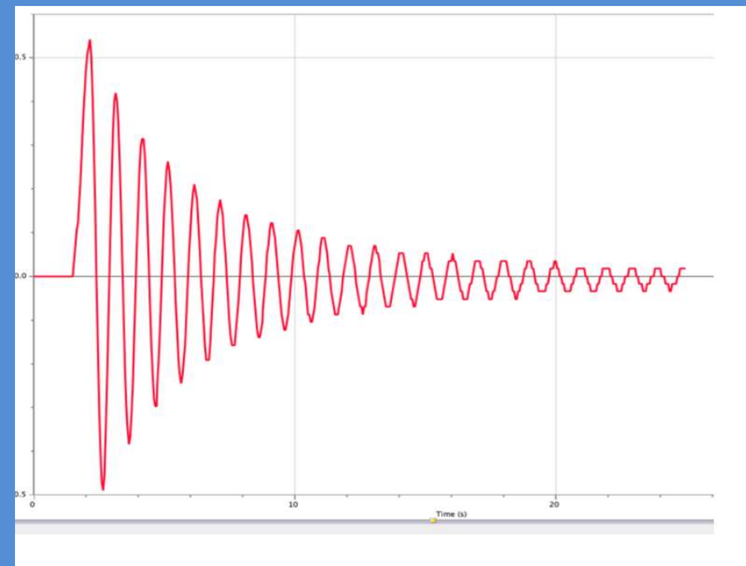
t is time (T).

Numerical

Finite Difference Method

Try x = 1, then x = 40, compare the difference and try again.

Through iterative attempts at solving the problem the difference between two answers is reduced to an acceptable level (convergence) – e.g. 15.03, or 14.96, etc



Solving groundwater flow numerically

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

$$\begin{aligned}
&CR_{i,j-1/2,k}\left(h_{i,j-1,k}-h_{i,j,k}\right) + CR_{i,j+1/2,k}\left(h_{i,j+1,k}-h_{i,j,k}\right)\\
&+ CC_{i-1/2,j,k}\left(h_{i-1,j,k}-h_{i,j,k}\right) + CC_{i+1/2,j,k}\left(h_{i+1,j,k}-h_{i,j,k}\right)\\
&+ CV_{i,j,k-1/2}\left(h_{i,j,k-1}-h_{i,j,k}\right) + CV_{i,j,k+1/2}\left(h_{i,j,k+1}-h_{i,j,k}\right)\\
&+ P_{i,j,k}\,h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\left(\Delta r_j\,\Delta c_i\,\Delta v_k\right)\frac{\Delta h_{i,j,k}}{\Delta t}.
\end{aligned}$$

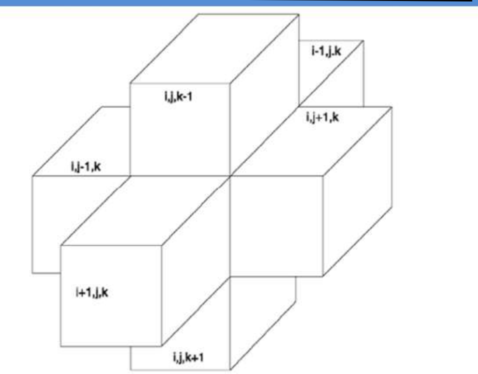
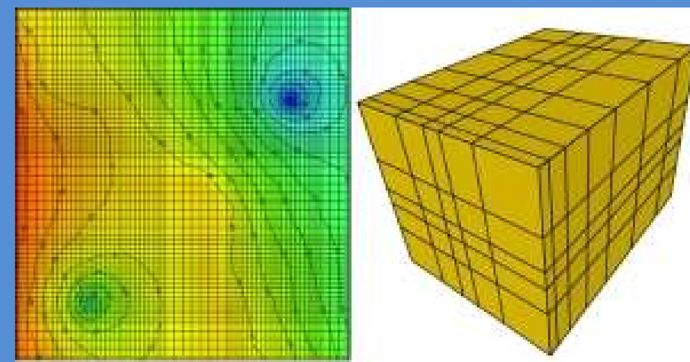
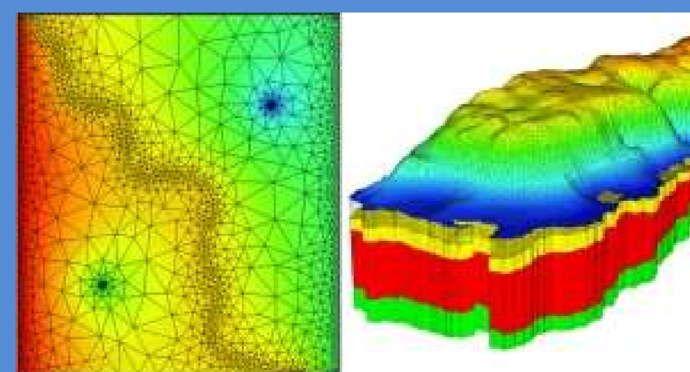


Figure 2–2. Indicies for the six adjacent cells surrounding cell i,j,k (hidden). (Modified from McDonald and Harbaugh, 1988.)

Numerical

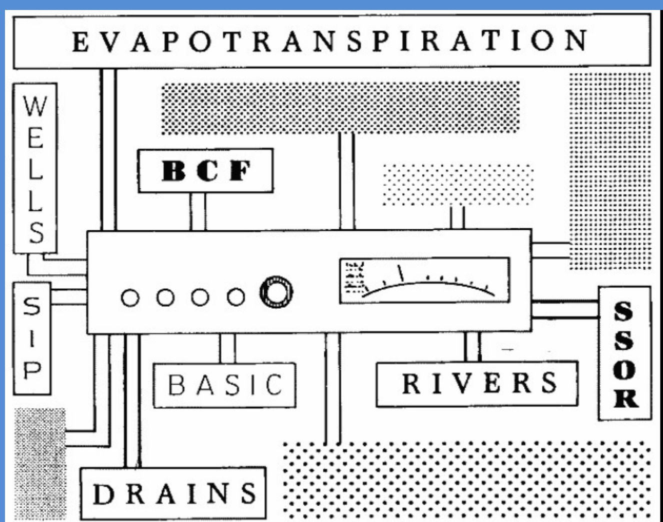
- Approaches complicated paramaterization with an iterative convergence approximation
- Typically a user-defined convergence criteria
- Approximation and Non-unique
- As discretization becomes more and more fine all numerical methods become instable (Habre, 2013)
- Example - MODFLOW
  - Finite difference approximation
  - Finite element
  - MODFLOW 1980's – current
  - MODFLOW USG

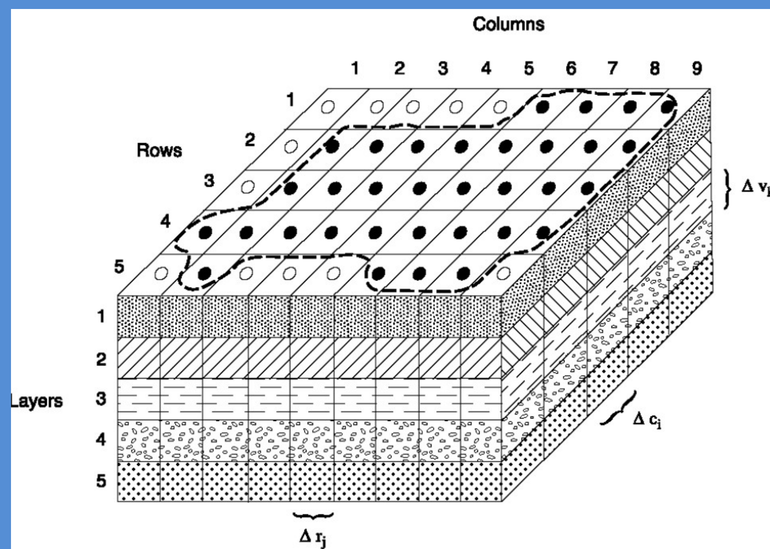


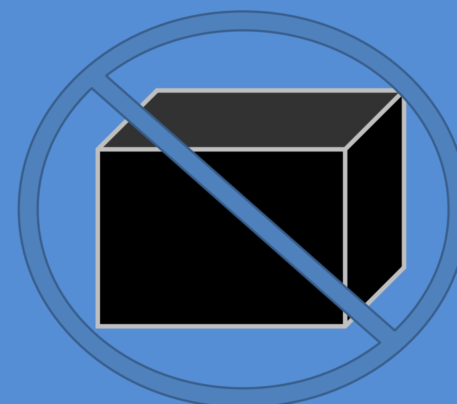


MODFLOW

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}$$

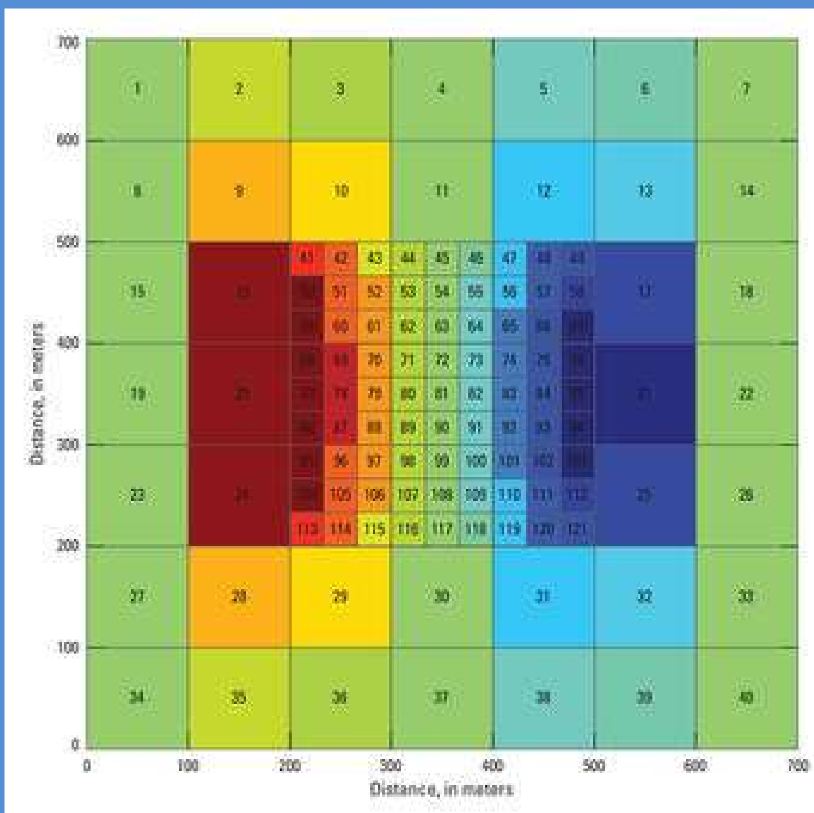


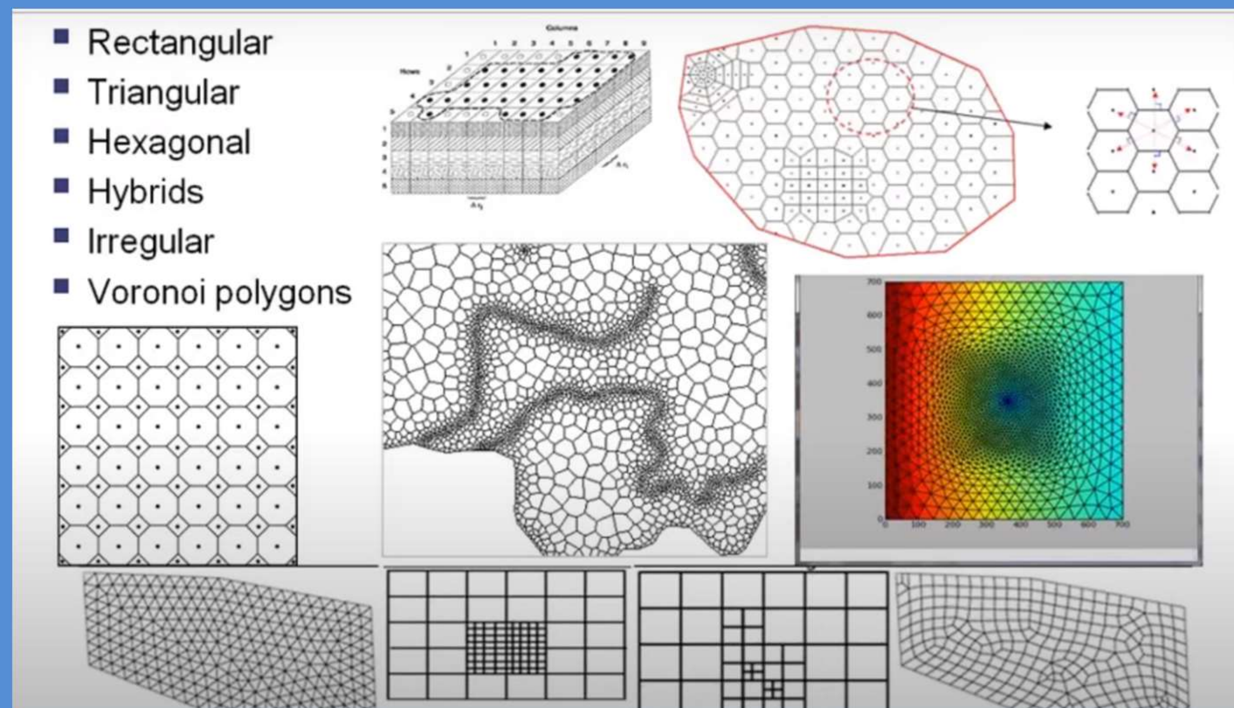




McDonald & Harbaugh (1983)

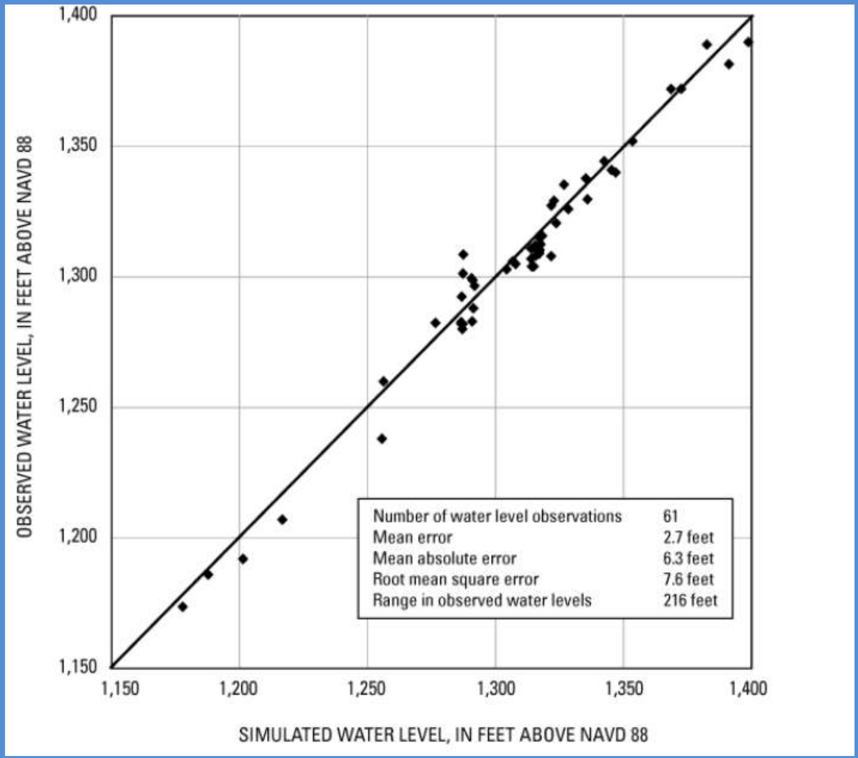
MODFLOW-USG


Distance, in meters
Distance, in meters
0
100
200
300
400
500
600
700

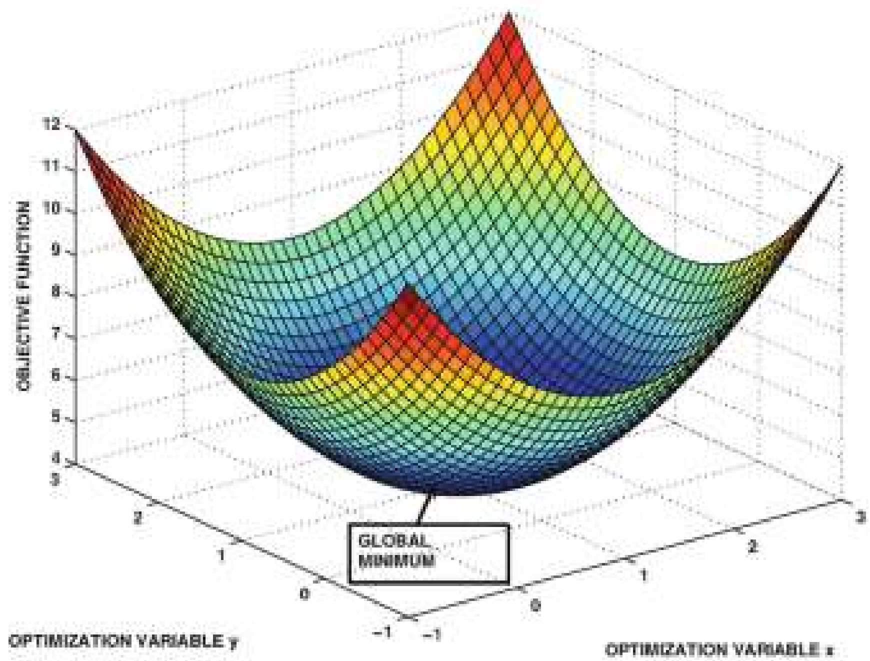

Rectangular
Triangular
Hexagonal
Hybrids
Irregular
Voronoi polygons

Model Calibration

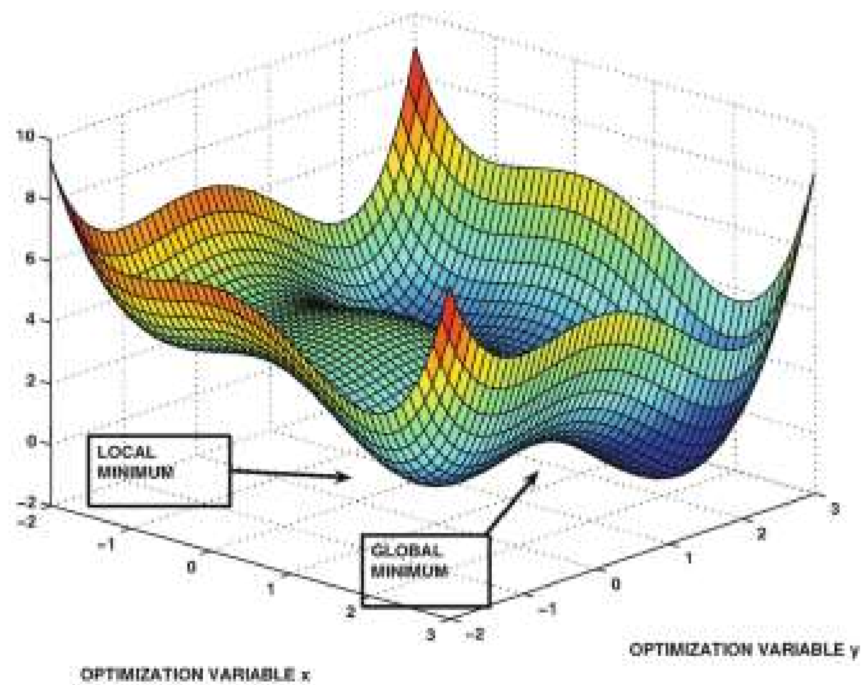
- Comparison of historical data to simulated results
- Systematic error reductions (objective function) through parameter value change iterations
- Various error reduction criteria
  - often reduced sum of squared residuals
  - No universal criteria



Non-Unique Solution

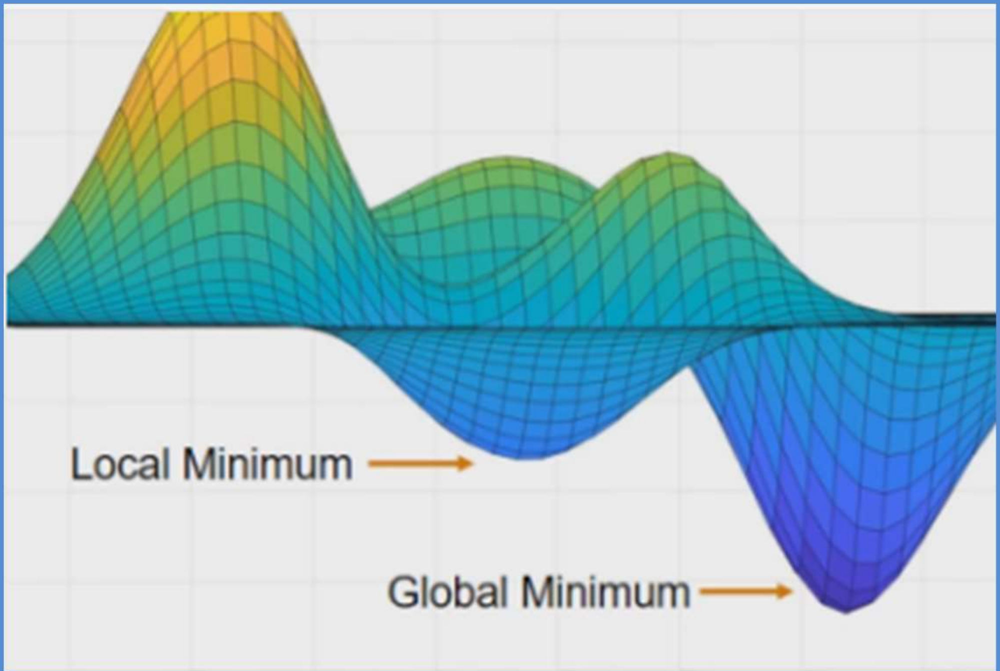


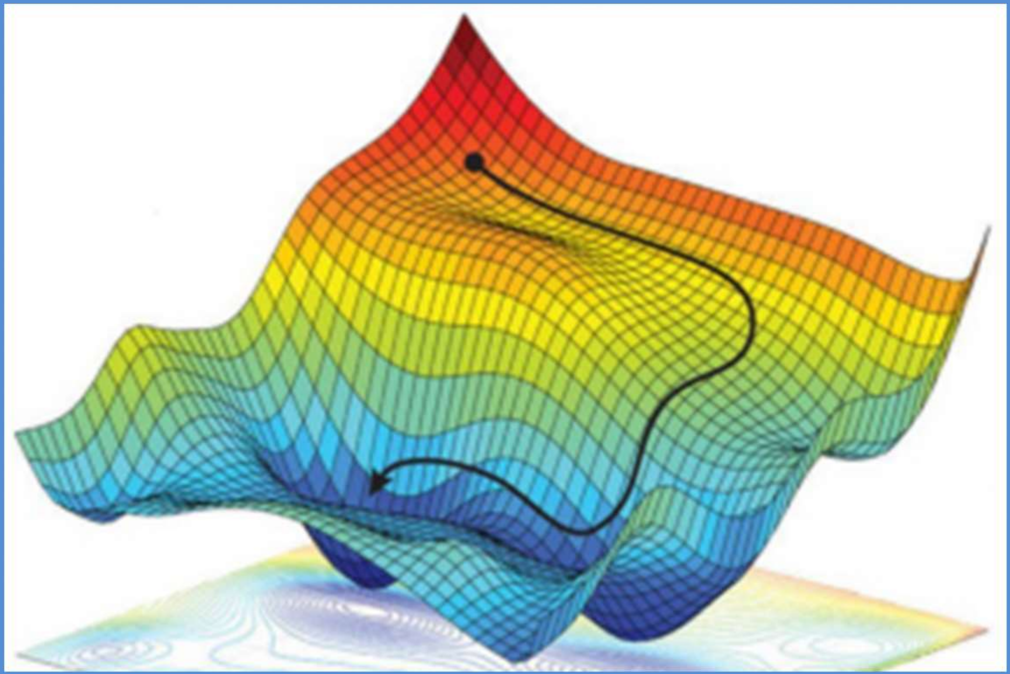
(a) Single global minimum



(b) Global and local minimum

Global Versus Local Minimum Objective Function





https://www.mathworks.com/products/global-optimization.html

https://vitalflux.com/convex-optimization-explained-concepts-examples/

PEST++

- Considerable enhancements
- Accessible
- Usable

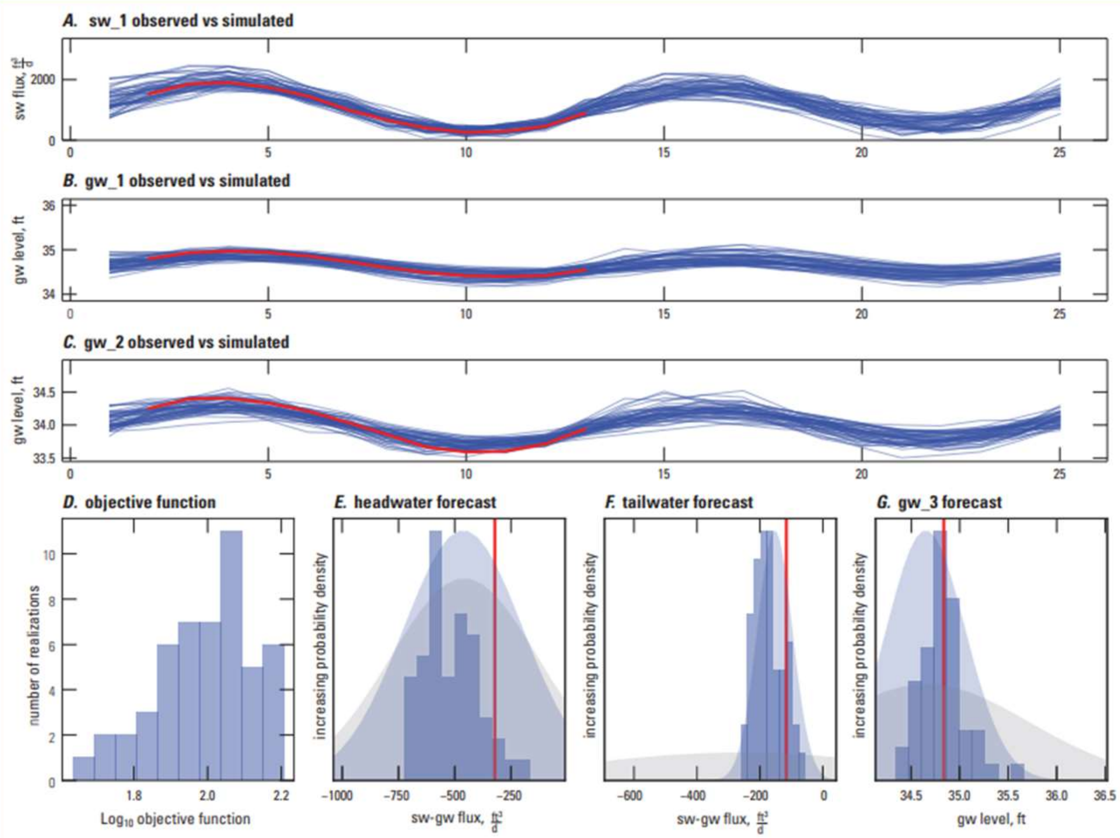


Figure 6. Summary of the advanced PESTPP-GLM analysis for the enhanced Freyberg model. *A*, *B*, and *C* show the observed (red) values versus simulated (blue) values for each of the posterior realizations. These results, taken with *D* (the objective function distribution for the filtered posterior ensemble) show a good level of agreement between the FOSM-based Monte Carlo realizations and the observed states used for history matching. *E*, *F*, and *G* show how both the FOSM prior (gray gaussian curves) and posterior (blue gaussian curves), as well as the Monte Carlo results (blue histograms), cover the true forecast values (red vertical bars). (sw, surface water; gw, groundwater, ft, feet; d, day; ft^3, cubic feet)

PESTPP-GLM Example 15

Source - https://pubs.usgs.gov/tm/07/c26/tm7c26.pdf

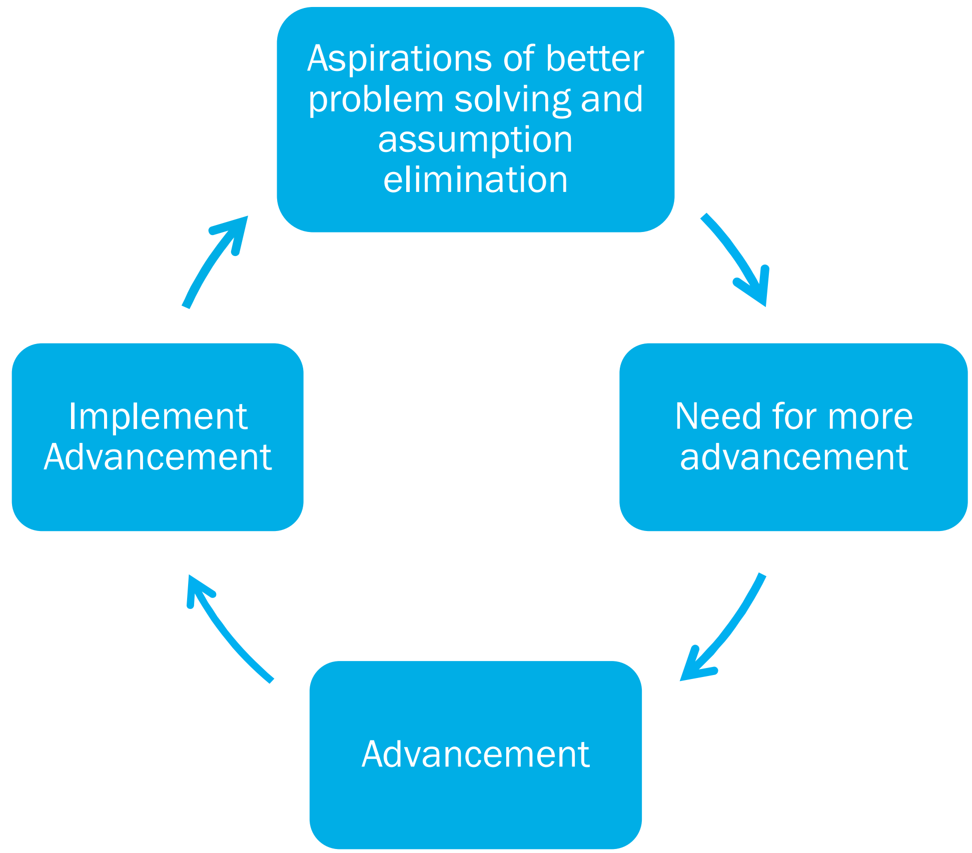
Site Example

PURPOSE

Why is this project relevant – What it means to you!

- Complicated: geological / hydrogeological / anthropogenetic environment
- Technological advancement cycling
    - Advancement begets advancement
- Demonstration of continual improvement in CSM – increasing resolution and studies
- Complexity can be resolved

Technological Advancement Cycling

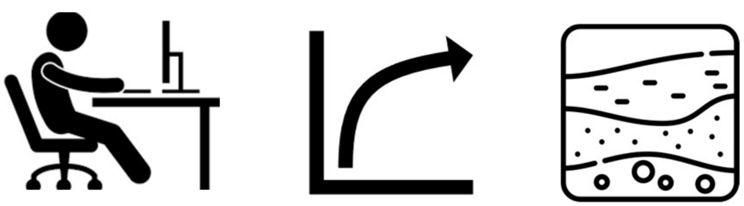


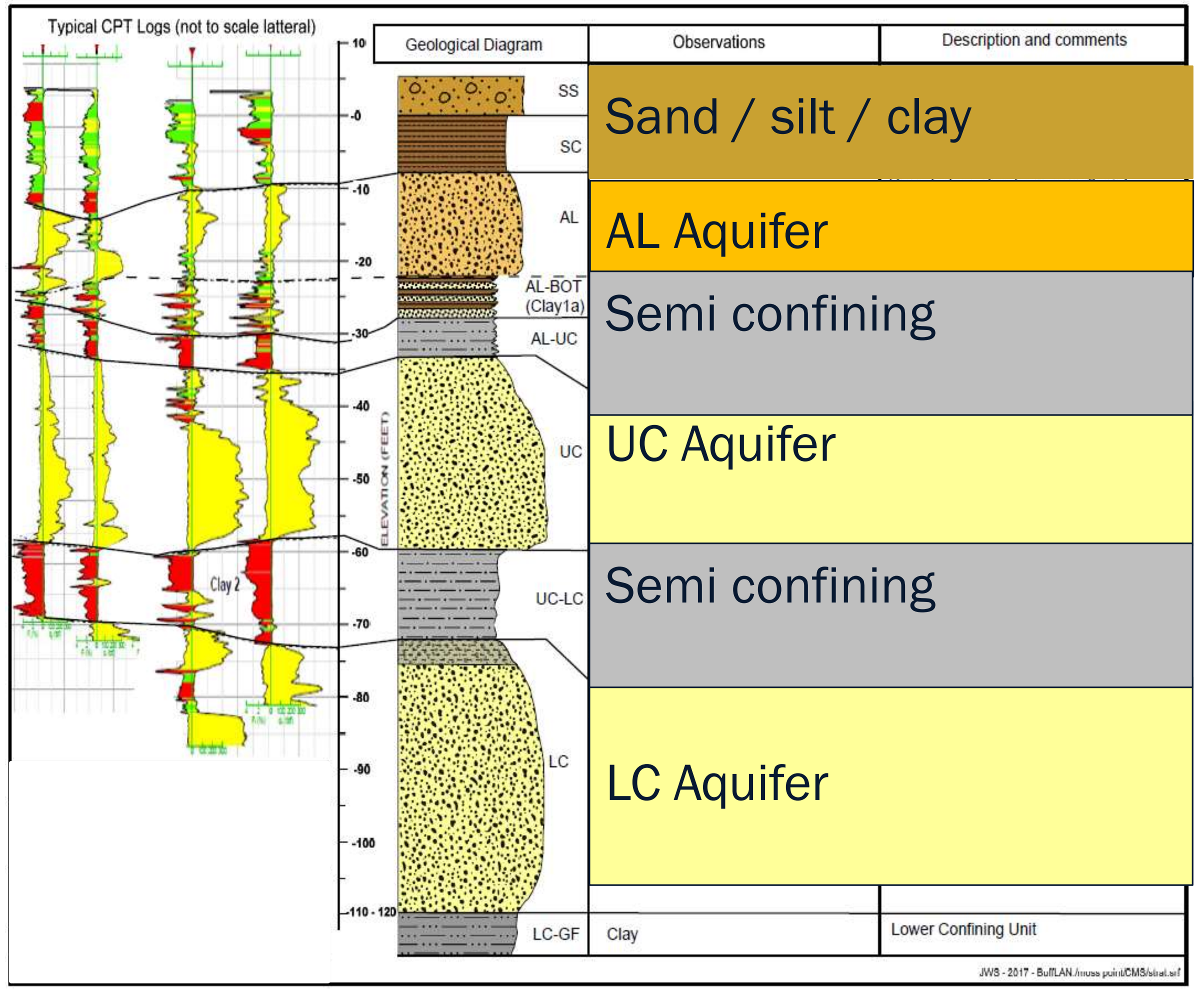
GEOLOGICAL / HYDROGEOLOGICAL / ANTHROPOGENETIC

- **Multilayered Aquifer System**
  - Semi-confining - discontinuous aquitards
- **Gradational transitions**
  - Marker horizons
  - Changes in redox
- **Downward gradients**
- **Tidal Influenced**
- **Density Driven Flow**
- **Static and pumping head data**

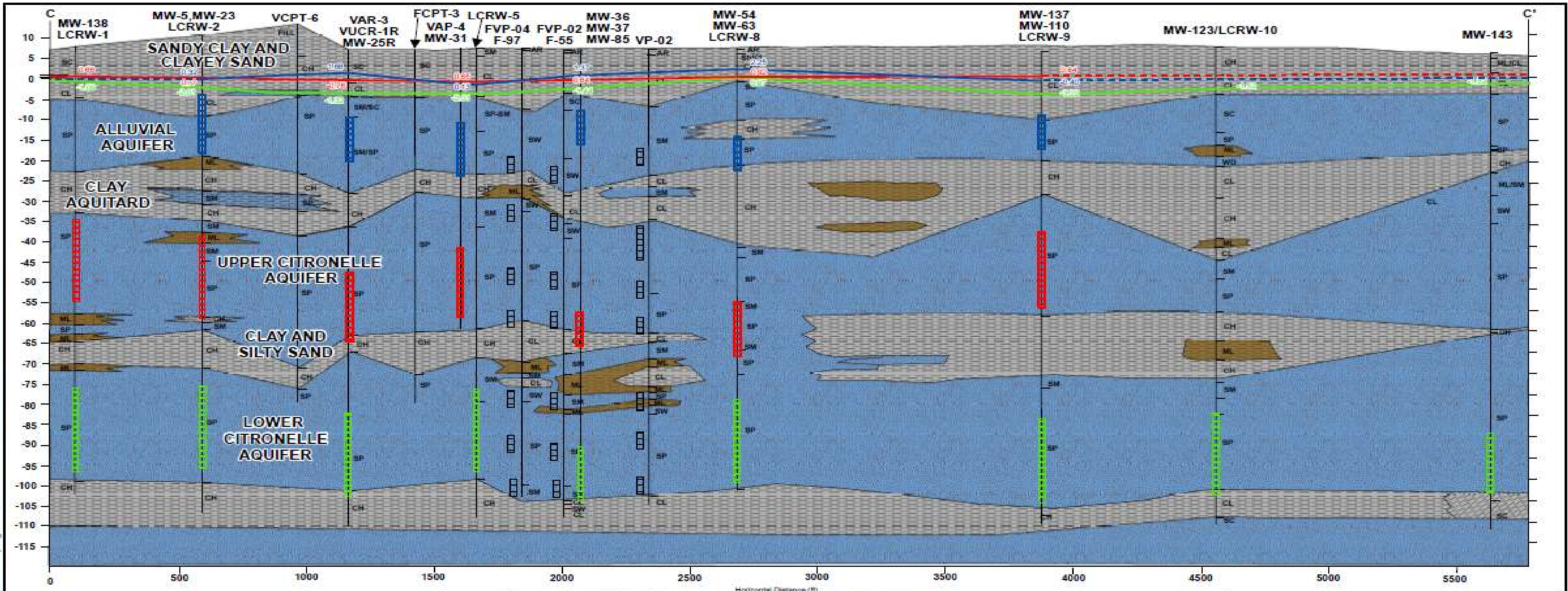
IMPROVE SITE CONCEPTUAL MODEL

- **Desire to move out of pump and treat**
- **Additional characterizations**
  - Highly detailed stratigraphic geological review
  - Geophysics – surface and downhole
  - Cone Penetration Testing
  - Tidal Studies
  - Pumping Tests
- **3D Modeling - SEAWAT**
- **Principle of Parsimony**





GEOLOGY



Cross-section Legend

- CLAY
- SILT
- WATER-BEARING SAND
- CLAYEY SAND

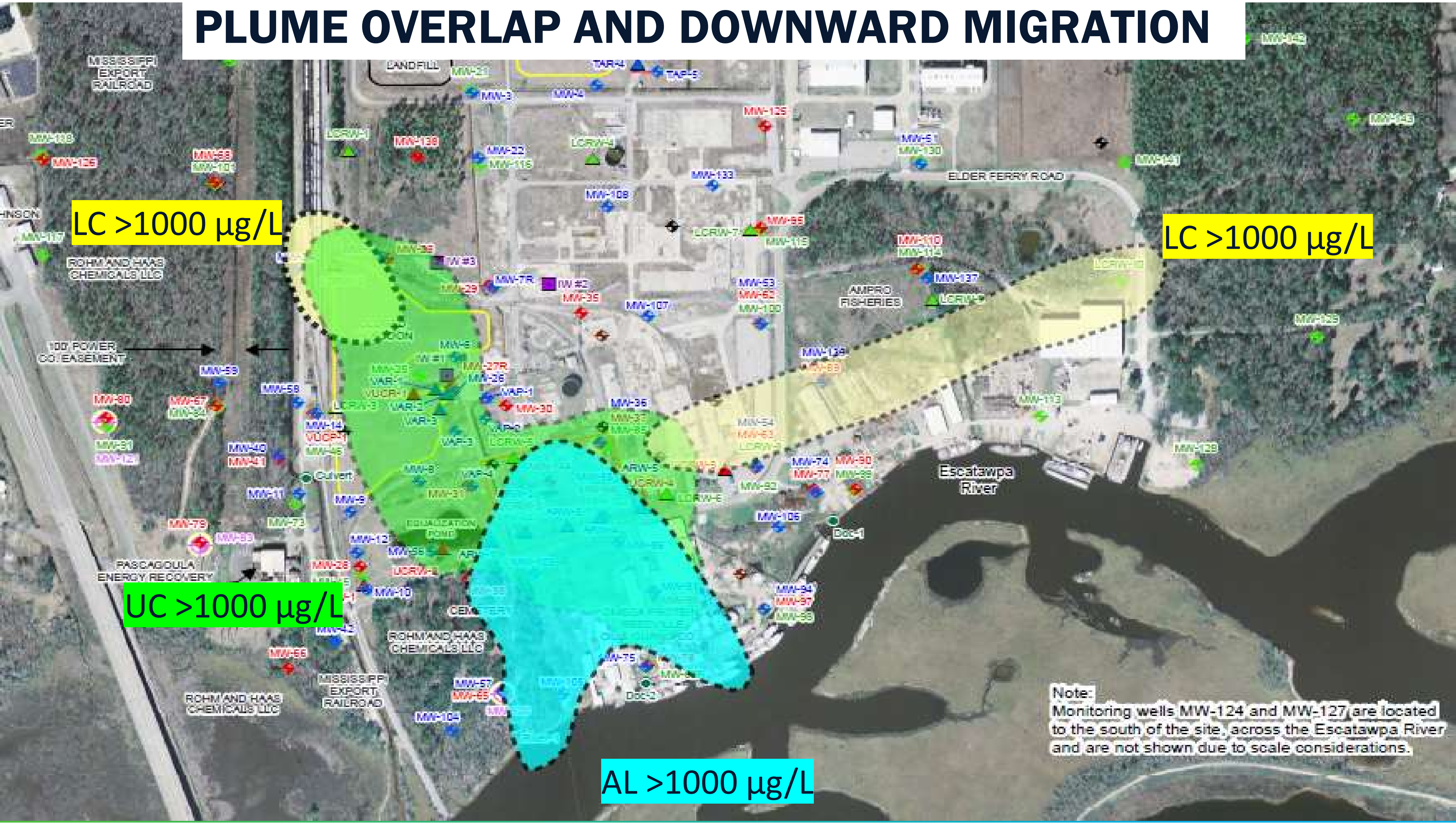
J = Qualified as estimated

1,200 TOTAL COC CONCENTRATION ug/L

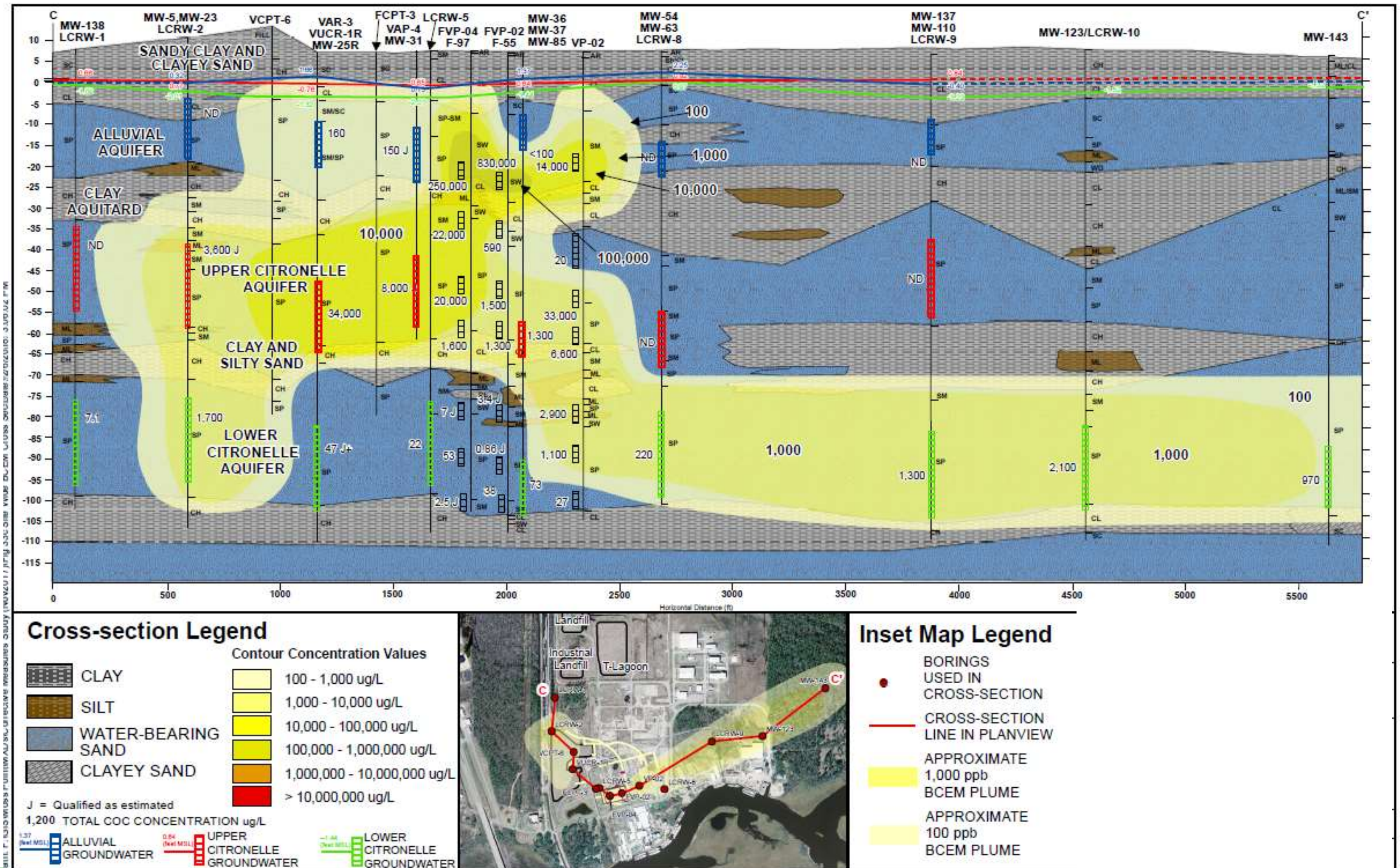
- 1.37 (feet MSL) ALLUVIAL GROUNDWATER
- 0.54 (feet MSL) UPPER CITRONELLE GROUNDWATER
- -1.44 (feet MSL) LOWER CITRONELLE GROUNDWATER

Path: F:\GIS\Moss Point\MXDs\Corrective Measures Study (Nov2017)\Fig 33a Site Wide BCEM Cross SecDate:12/7/2018 7:12:49 PM

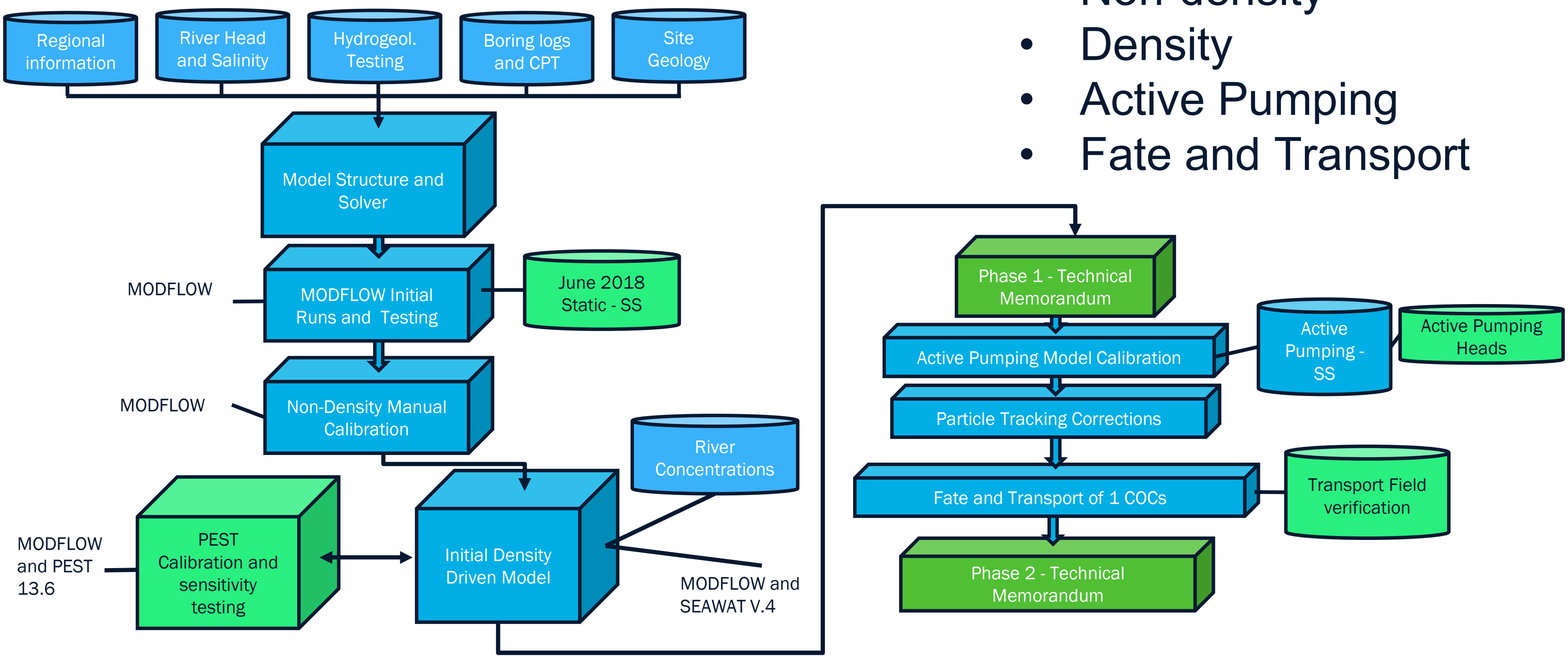
PLUME OVERLAP AND DOWNWARD MIGRATION



PLUME OVERLAP AND DOWNWARD MIGRATION



WORKFLOW



MULTIPLE CALIBRATIONS

- Non-density
- Density
- Active Pumping
- Fate and Transport

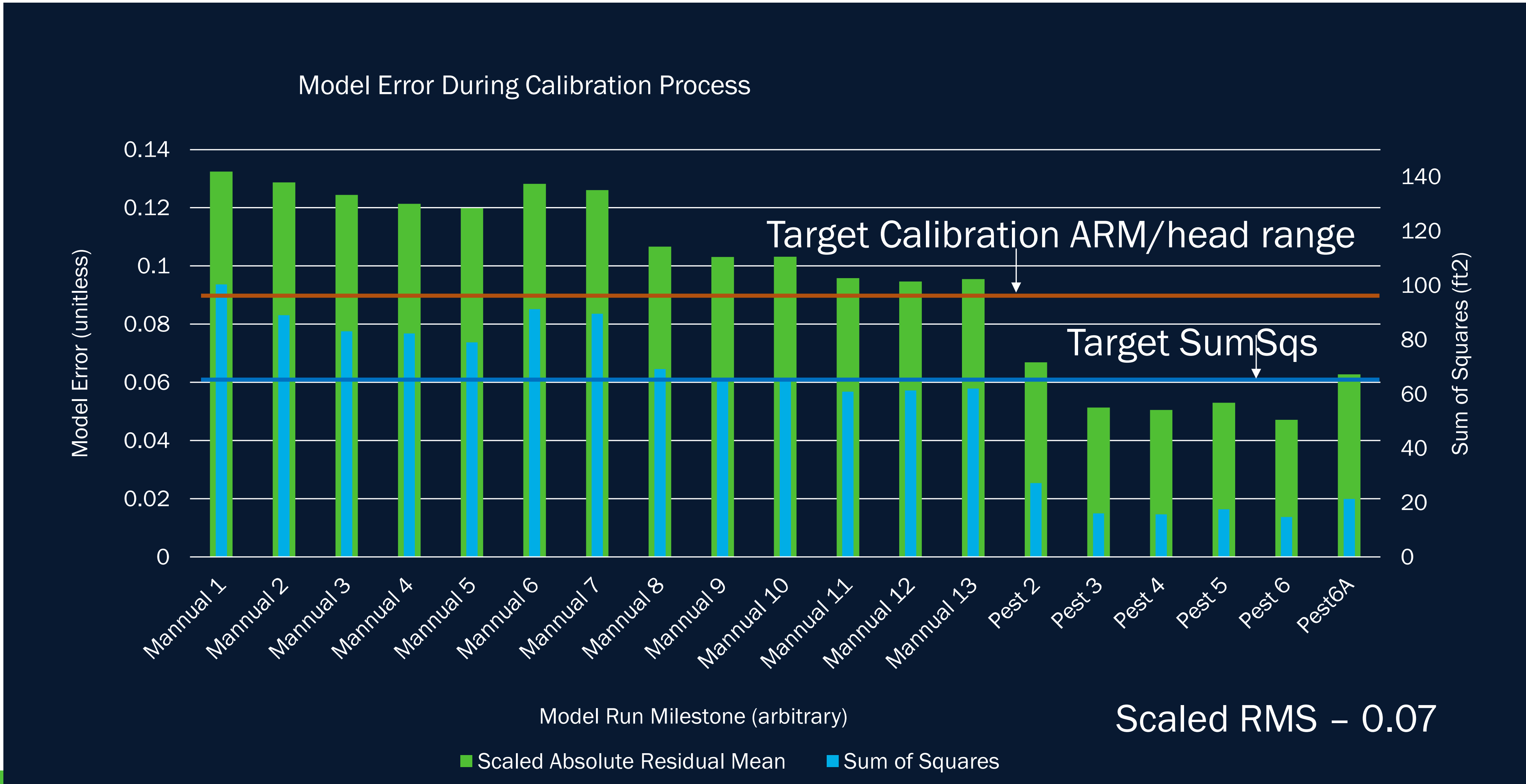
Stress Periods Descriptions Site Numerical SEAWAT Model

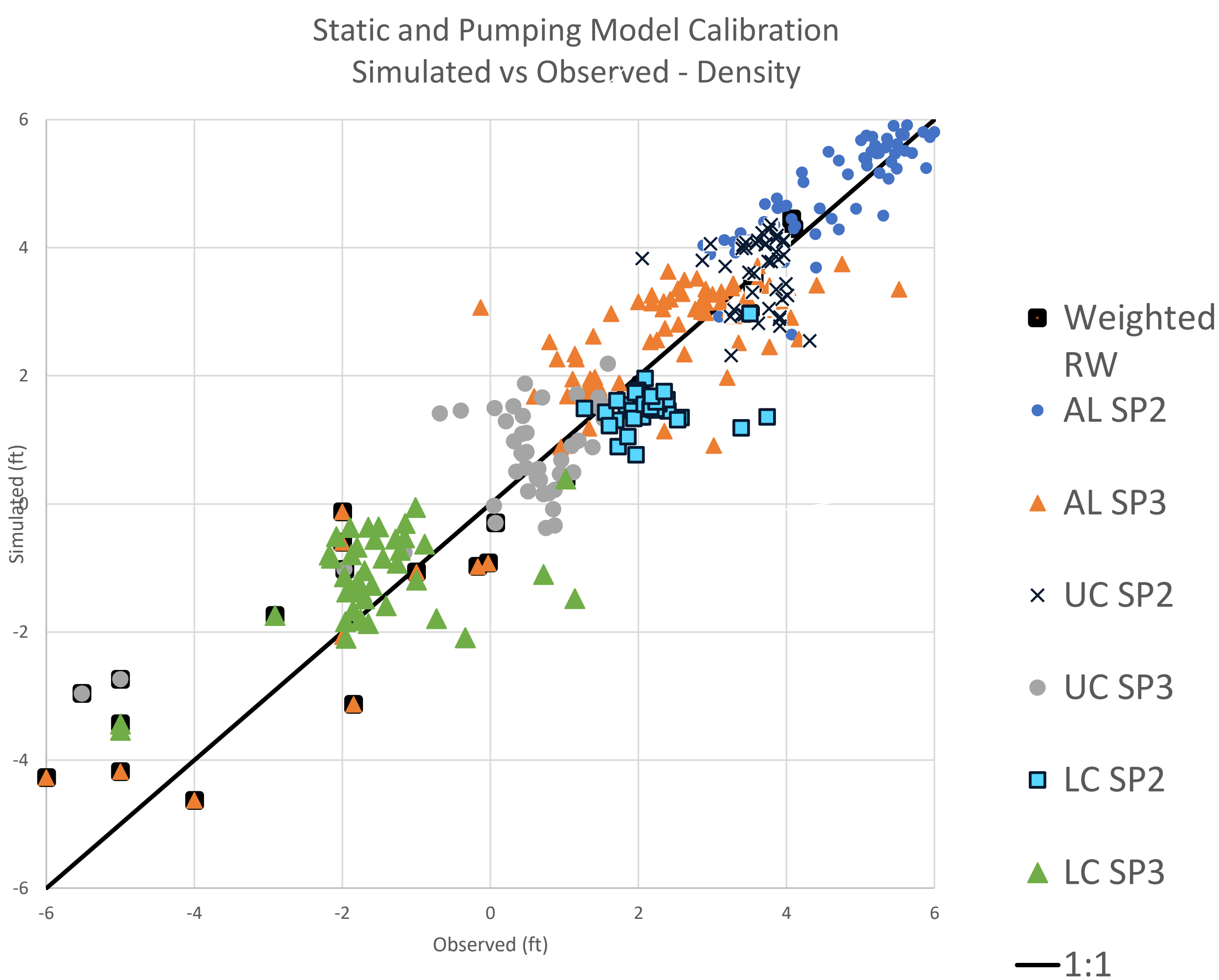
1) **Long Term Natural Conditions**
- 500 Years
- Development of density wedge
- Calibration Point

2) **Site historical operations**
- ~42 years
- Similar Non-pumping conditions
- Beginning of release

3) **Initiate Pump and Treat**
- 12 years – 2006 - 2018
- Pumping from three aquifers
- Recovery of plume
- Calibration point

CALIBRATION EXAMPLE - TRIAL / ERROR AND PEST



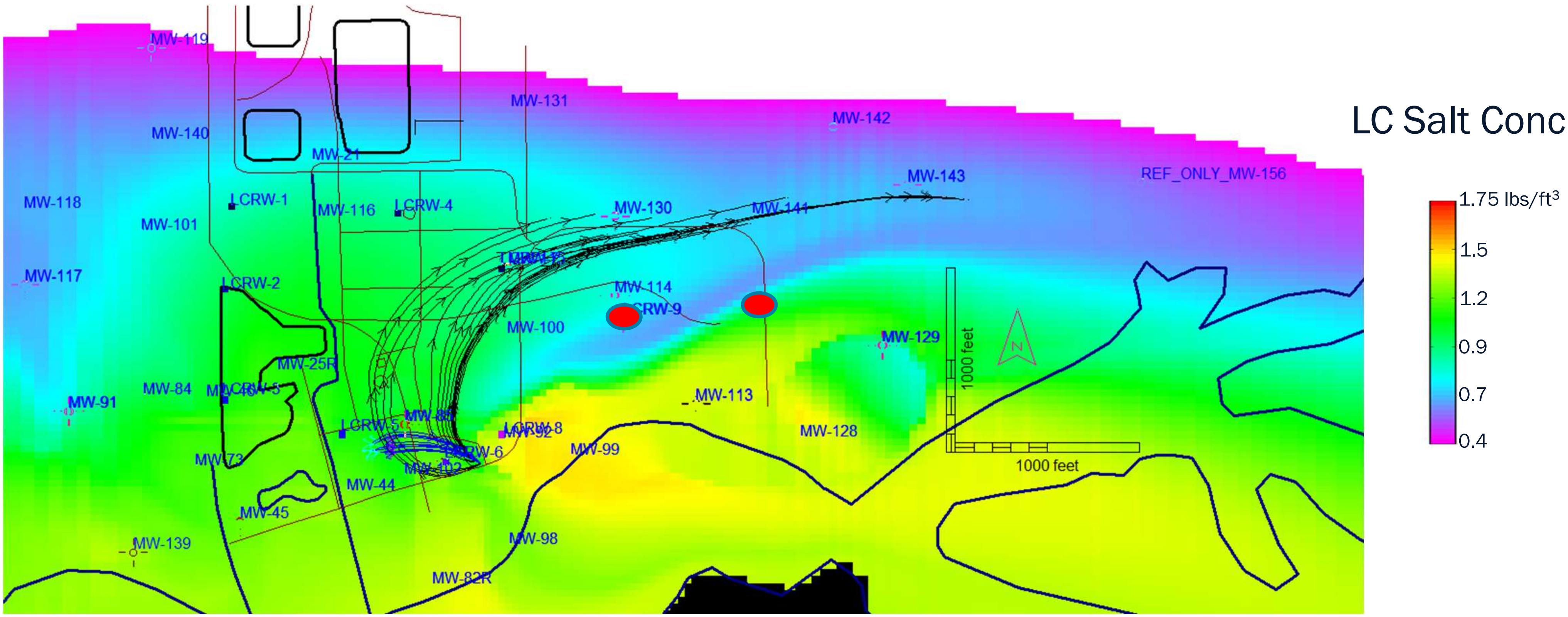


Calibration Statistics	
Residual Mean	-0.12
Absolute Residual Mean	0.64
Residual Std. Deviation	0.81
Sum of Squares	221.04
RMS Error	0.82
Min. Residual	-3.20
Max. Residual	2.62
Number of Observations	327.00
Range in Observations	12.23
Scaled Residual Std. Deviation	0.07
Scaled Absolute Residual Mean	0.05
Scaled RMS Error	0.07
Scaled Residual Mean	-0.01

Static and Pumping Calibrations Pumping Calibration with Density

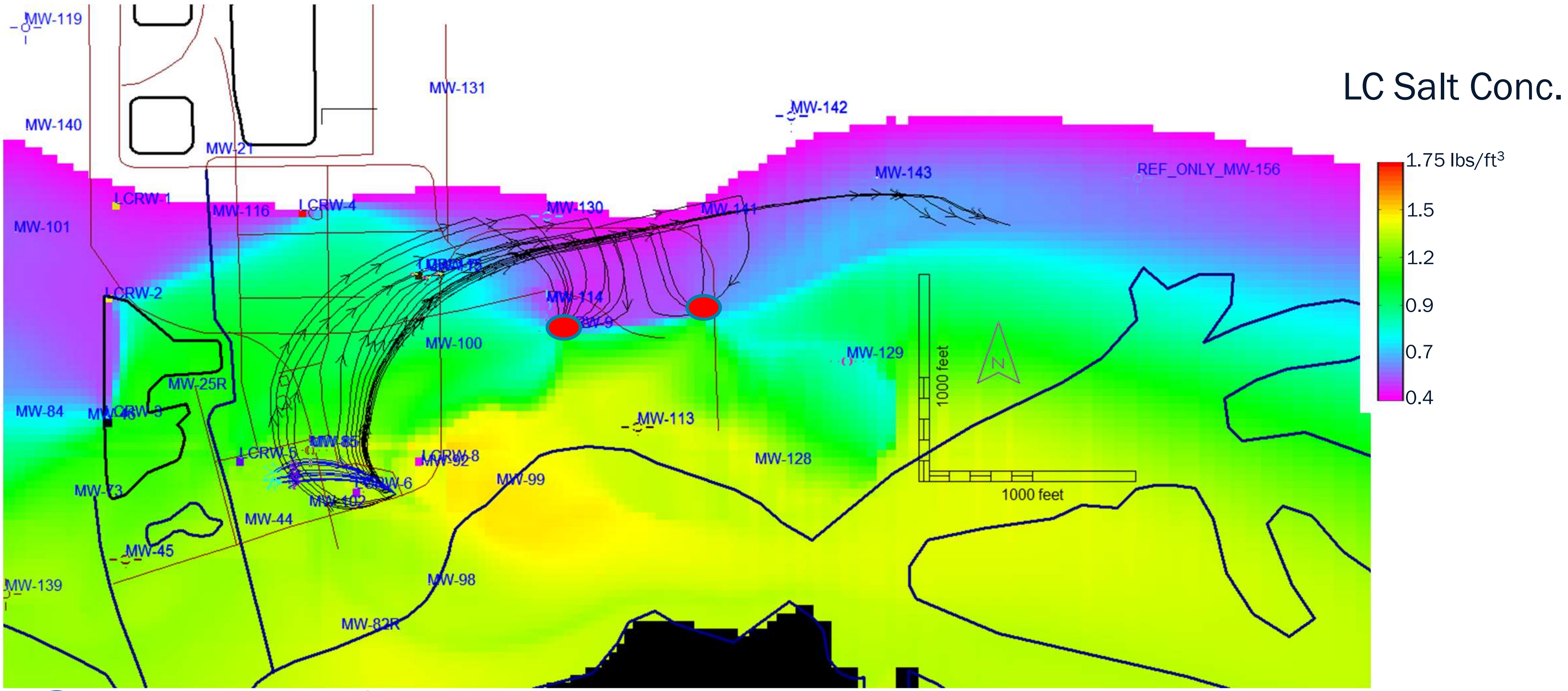
Numerical SEAWAT Model

Salt Concentrations 500 years with MODPATH Particles after non-pumping period (42 year)

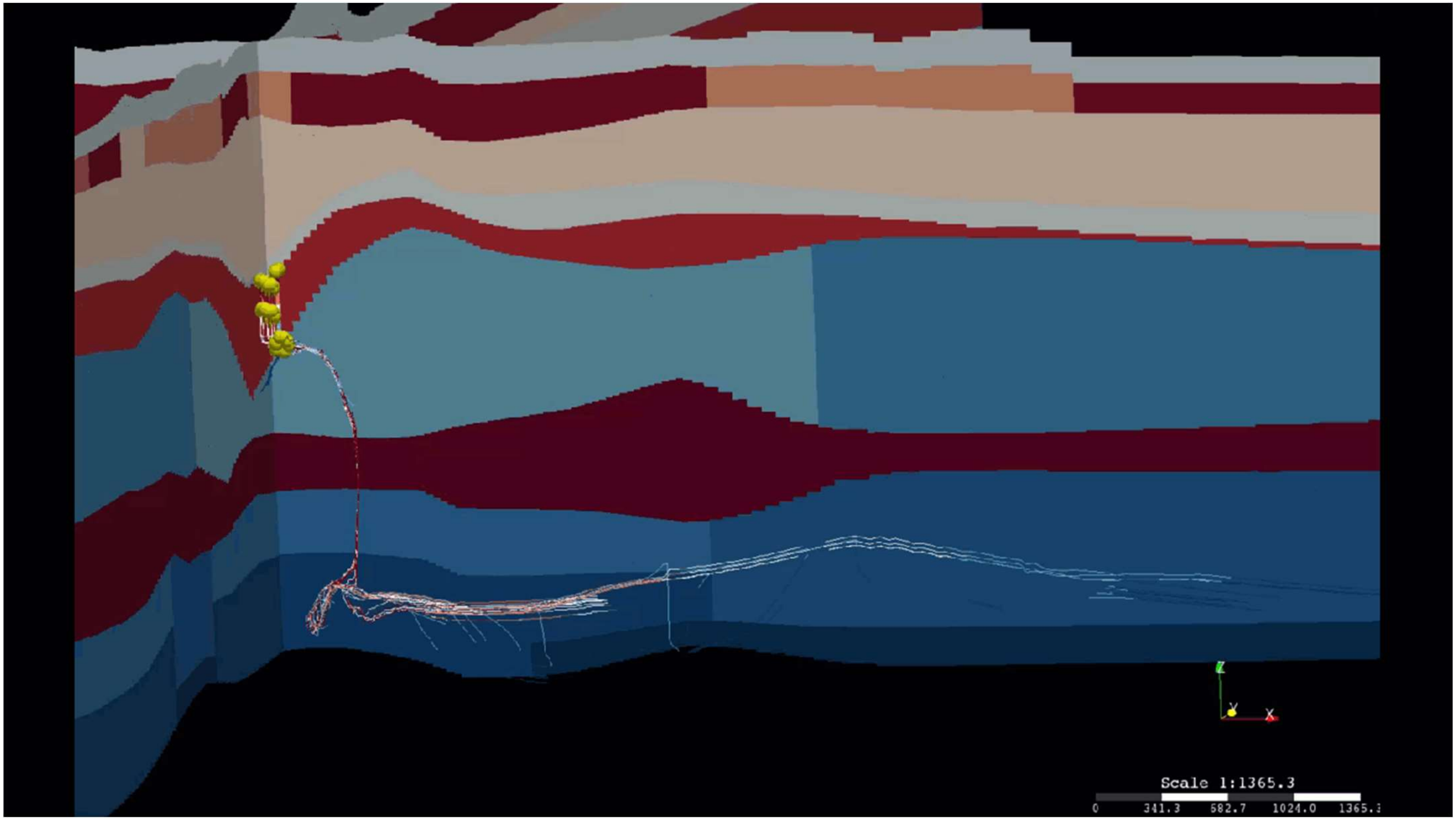


Recovery well of interest

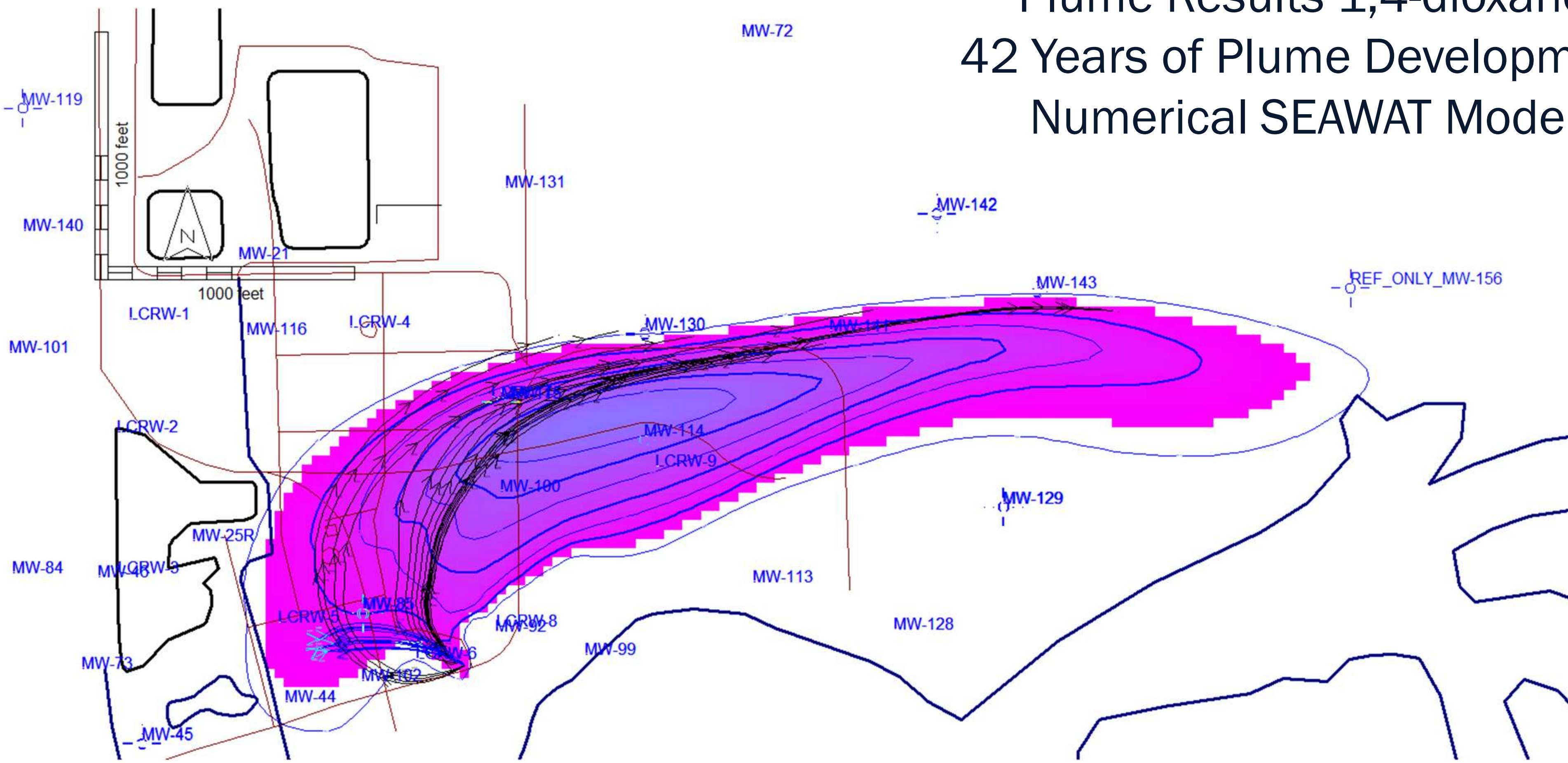
Salt Concentrations (500 years) with MODPATH Particles after non-pumping period (42 years) / pumping conditions (12 year)



Recovery well of interest

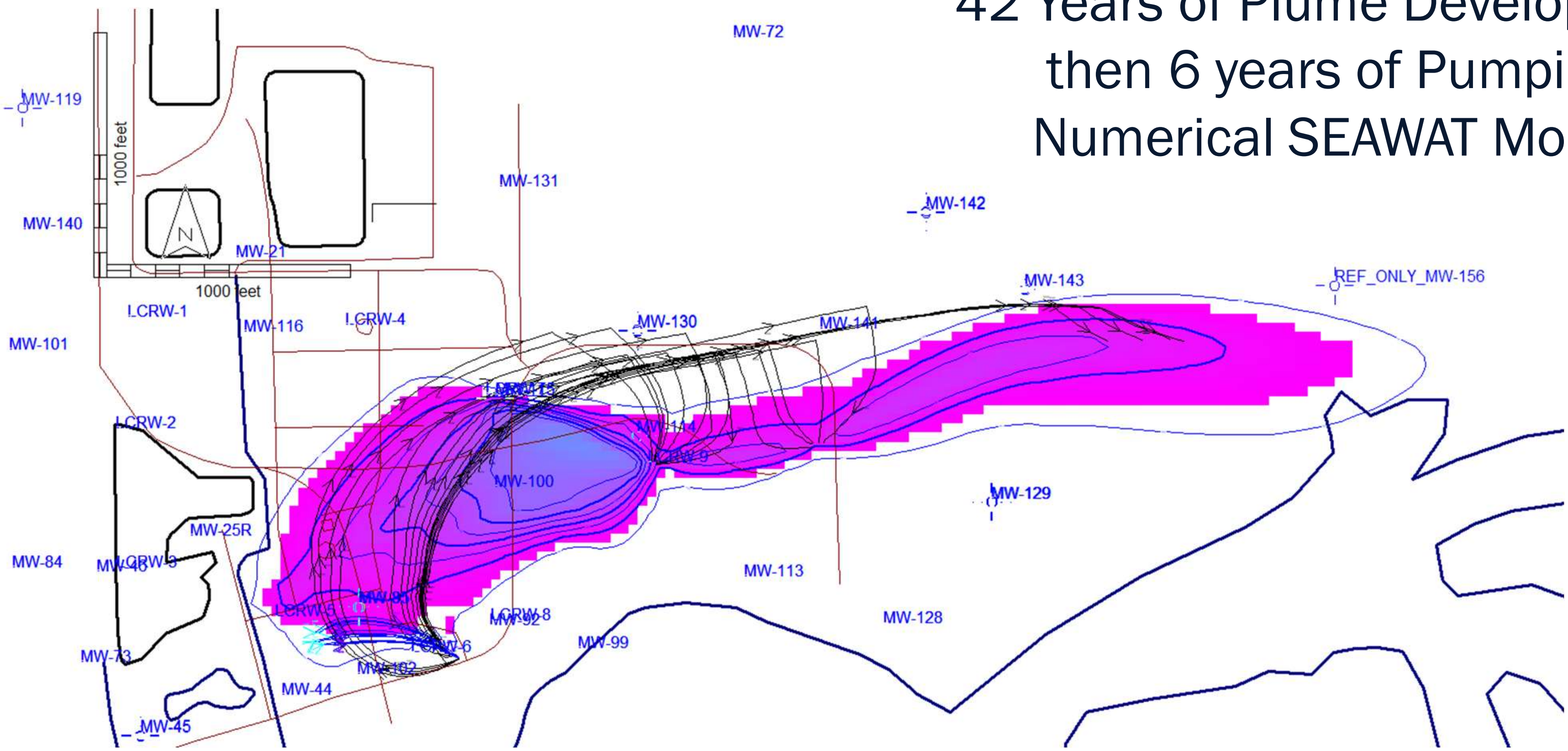

Scale 1:1365.3
0
341.3
682.7
1024.0

Plume Results 1,4-dioxane
42 Years of Plume Development
Numerical SEAWAT Model



Notes:
Color shading minimum is 5 µg/L
Minimum Contour 10 µg/L

Plume Results 1,4-Dioxane
42 Years of Plume Development then 6 years of Pumping
Numerical SEAWAT Model

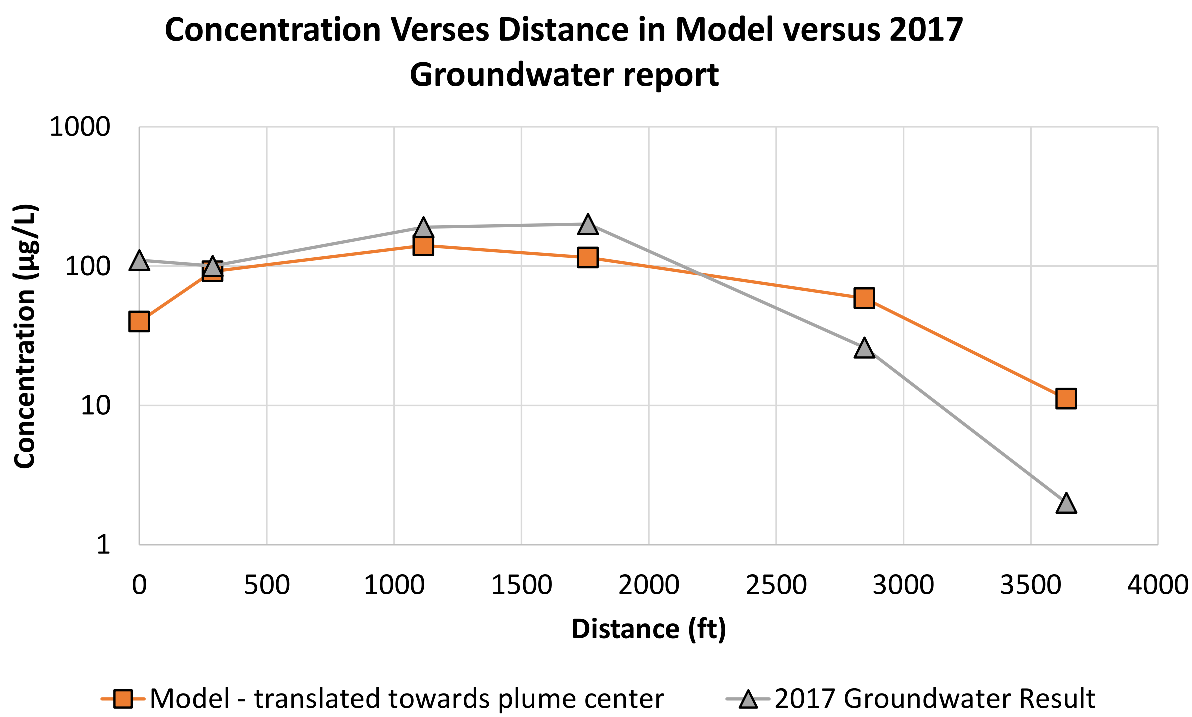


Notes:
Color shading minimum is 5 µg/L
Minimum Contour 10 µg/L

6 years of recovery represents half of the total system time, noting that early years rates were lower and LCRW-10 was not online

Evolution of groundwater modeling allows for:

- More detailed geological structures
- Fate and transport in complex flow regimes
- Advanced thought processes and site analyses



Advancement begets advancement

QUESTIONS

1) What is the purpose of calibration?

2) Why is understanding tidal influence on groundwater levels important?

3) What is PEST?

4) Is groundwater modeling witchcraft?

5) What is the Principle of Parsimony?

THANKS!

QUESTIONS?

Unraveling Complexity through Fate and Transport Numerical Simulations in a Tidally-Influenced Heterogenous, Multi-System, Density Driven Regime

Presentation date: January 26, 2023

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