Primer on Modeling

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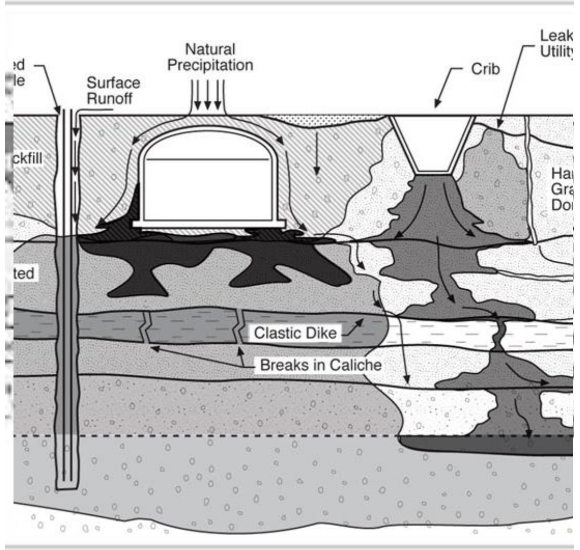
Hanford Hydrogeologist

Oregon Hanford Cleanup Board March 2019 Meeting



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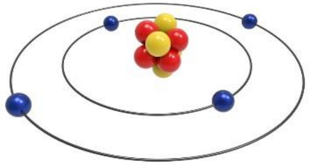
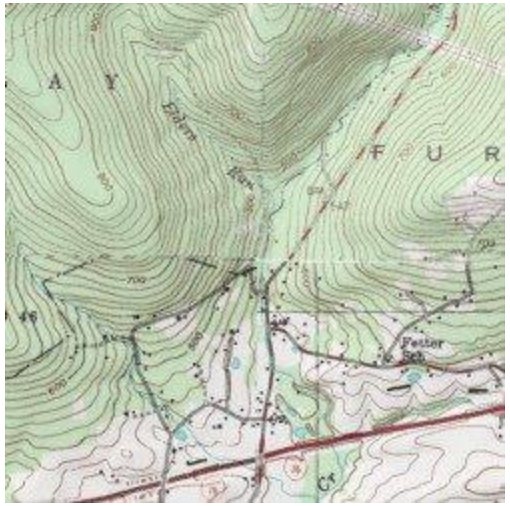
Roadmap

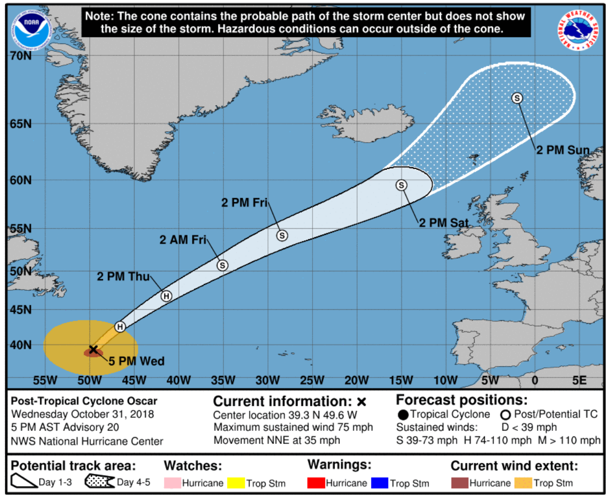
- What a model is
- How a model gets built
- What makes a good model
- Can models be abused
- Hanford

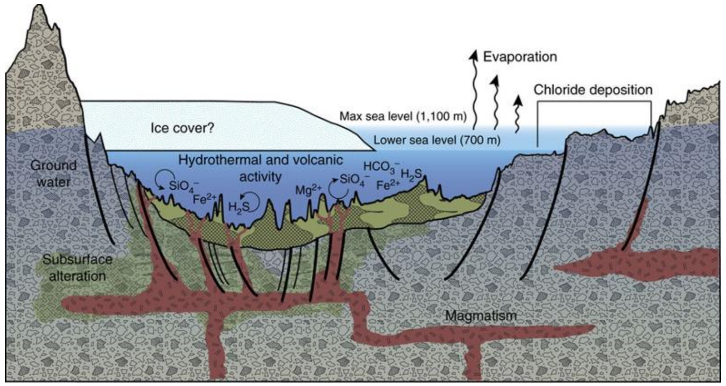


WHAT IS A MODEL?

- A simplified description of an existing physical system
- A description or analogy used to help visualize something that can not be directly observed

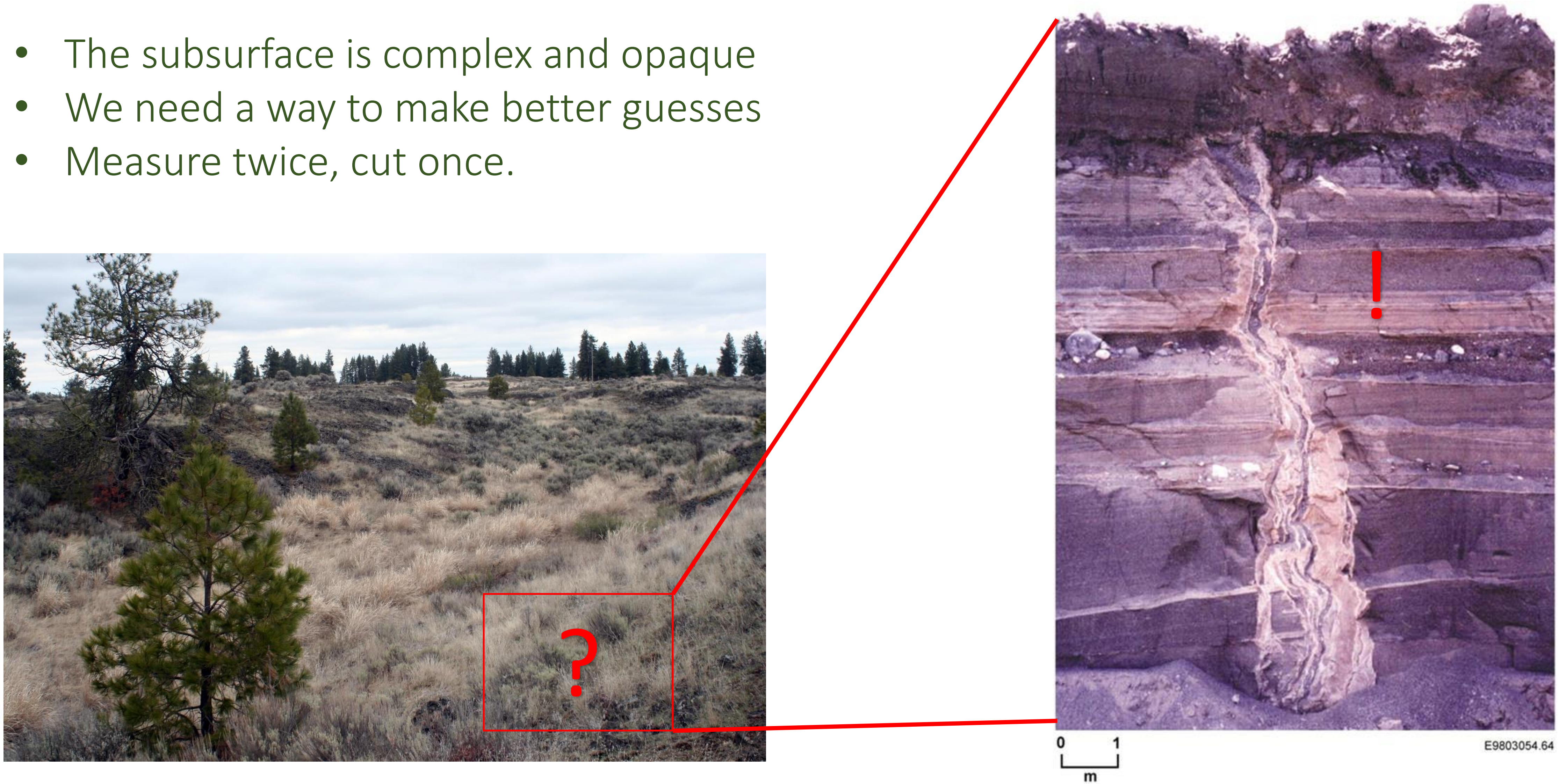






WHY A MODEL?

- The subsurface is complex and opaque
- We need a way to make better guesses
- Measure twice, cut once.



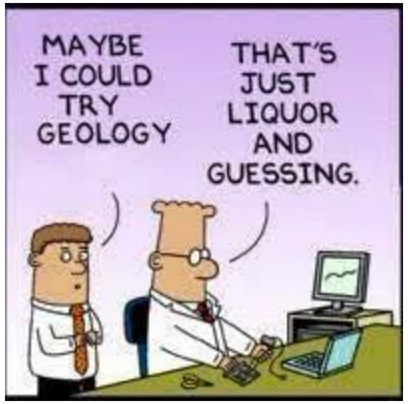
WHAT KIND OF MODEL?

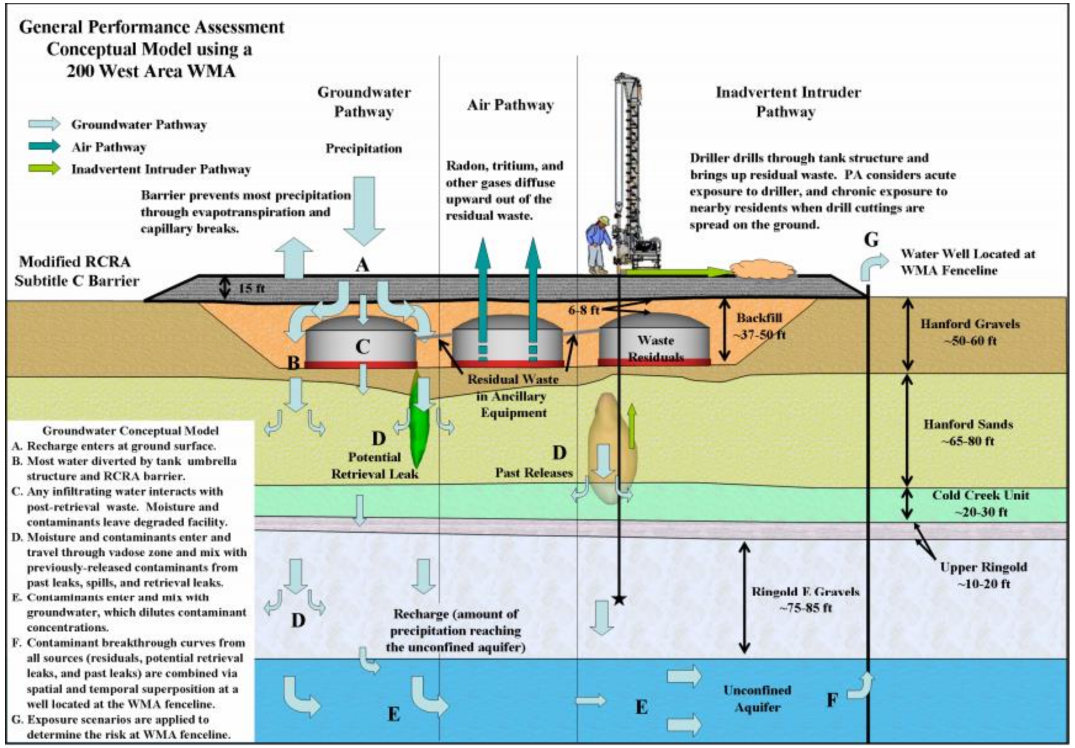
- How much do you know?

- How precise an answer do you need?

CONCEPTUAL MODEL

- Use past experience and data to guess





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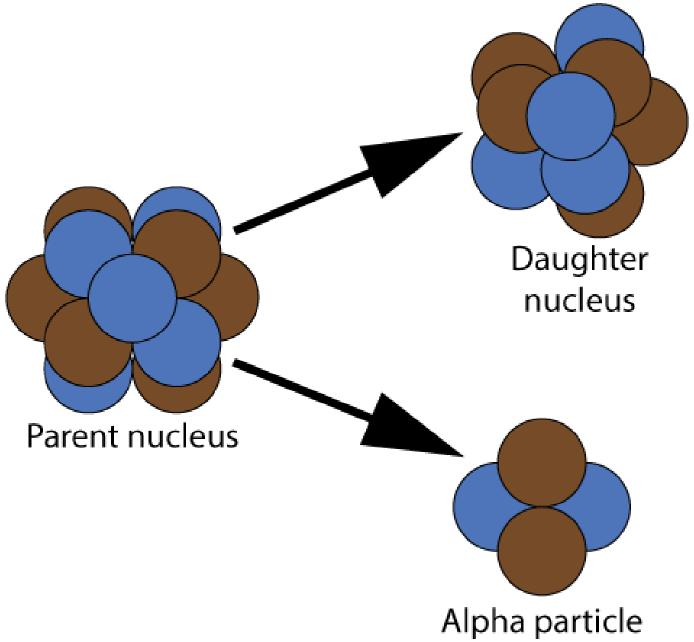
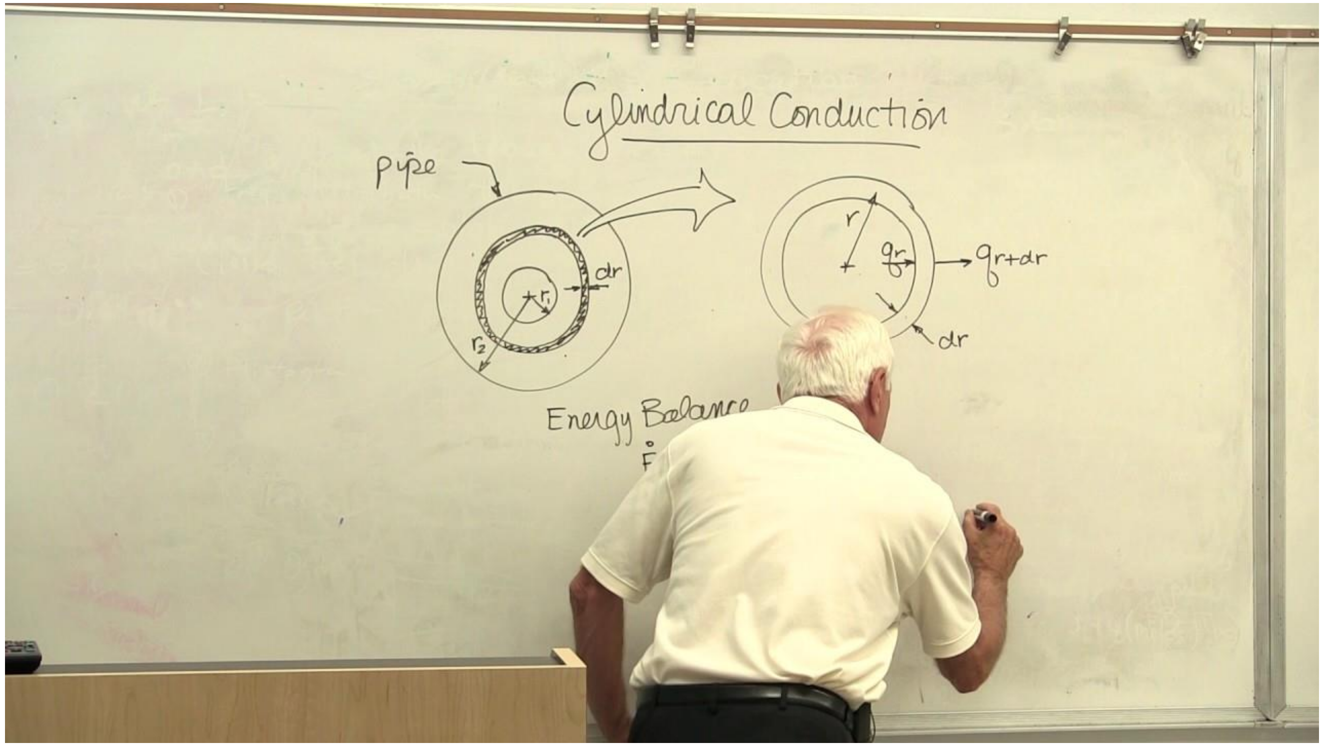
ANALYTICAL MODEL

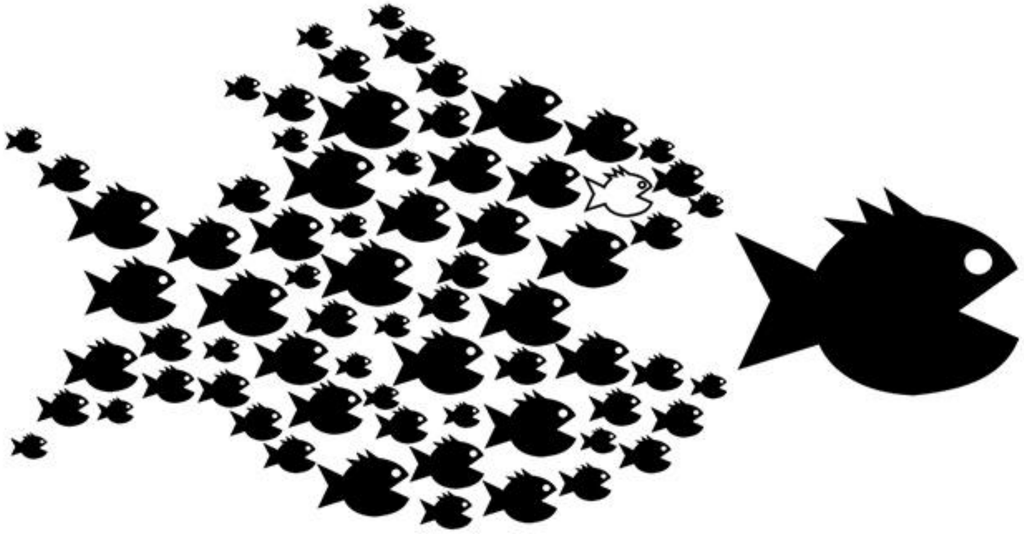
- Use “perfect” equation to know





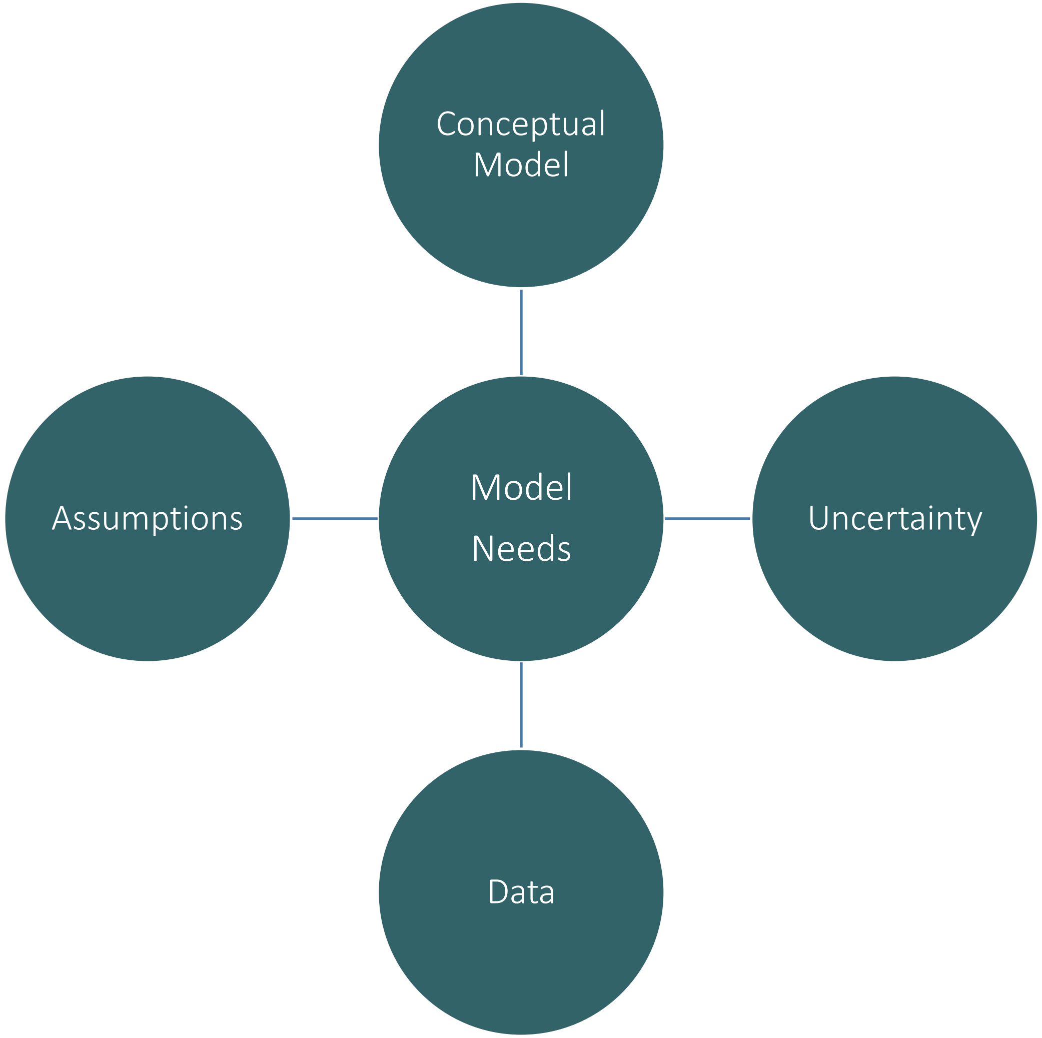
NUMERICAL MODEL

- Use brute computations to estimate



HOW WRONG IS YOUR MODEL?

- Numerical Models are never "true" All models are wrong, but some are useful
- The model is one representation of a potential outcome, given the assumptions, data, and the underlying conceptual model.



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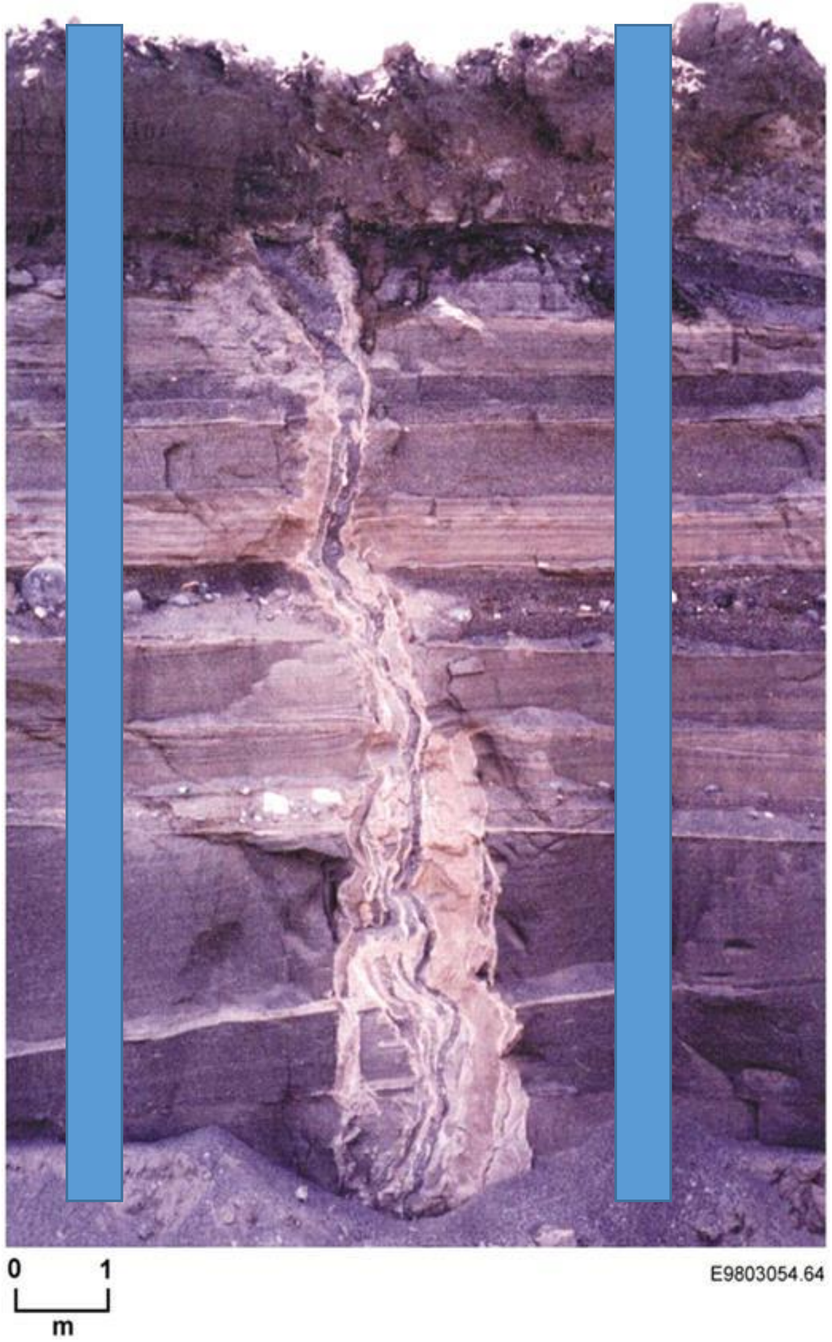

Building Blocks (discretizing the world)

STEP ONE – COLLECT SOIL/ROCK DATA

Drill cuttings

Split Spoon every 5’

Continuous logging

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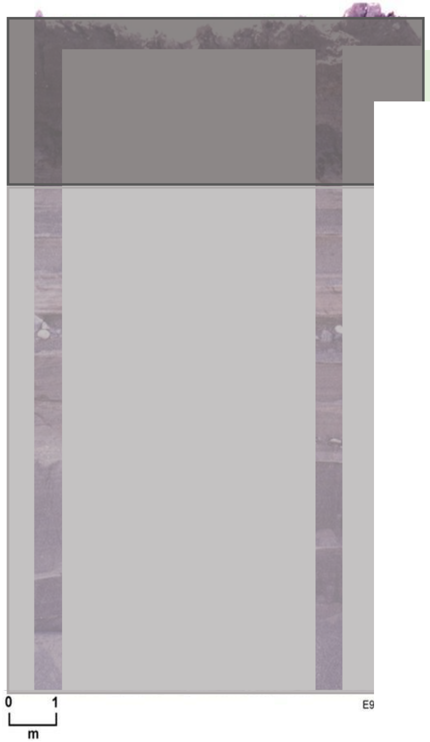
STEP ONE – COLLECT SOIL/ROCK DATA

Drill cuttings



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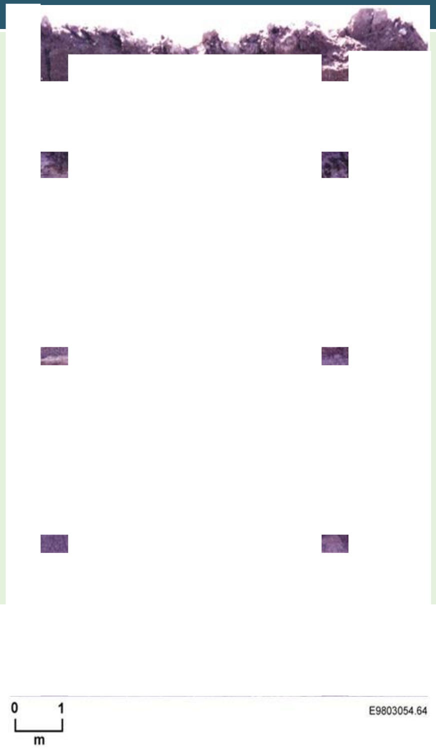
STEP ONE – COLLECT SOIL/ROCK DATA

Split Spoon every 5’



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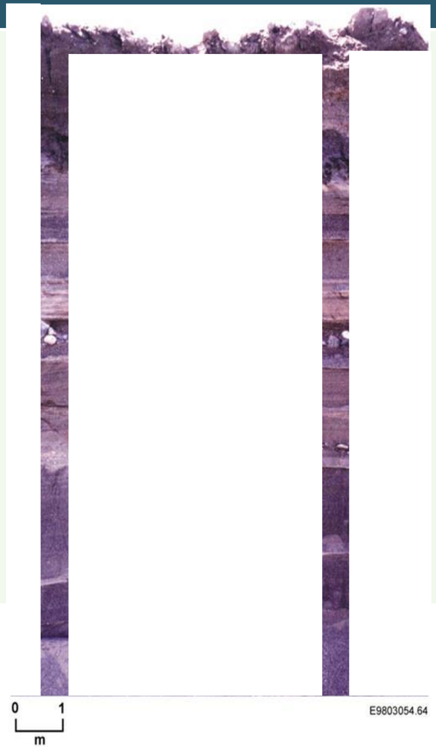
STEP ONE – COLLECT SOIL/ROCK DATA

Continuous logging



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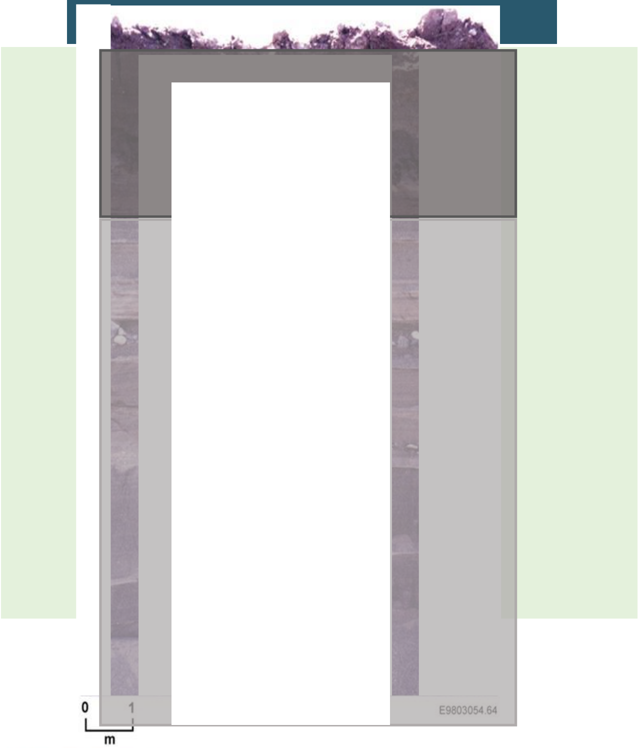
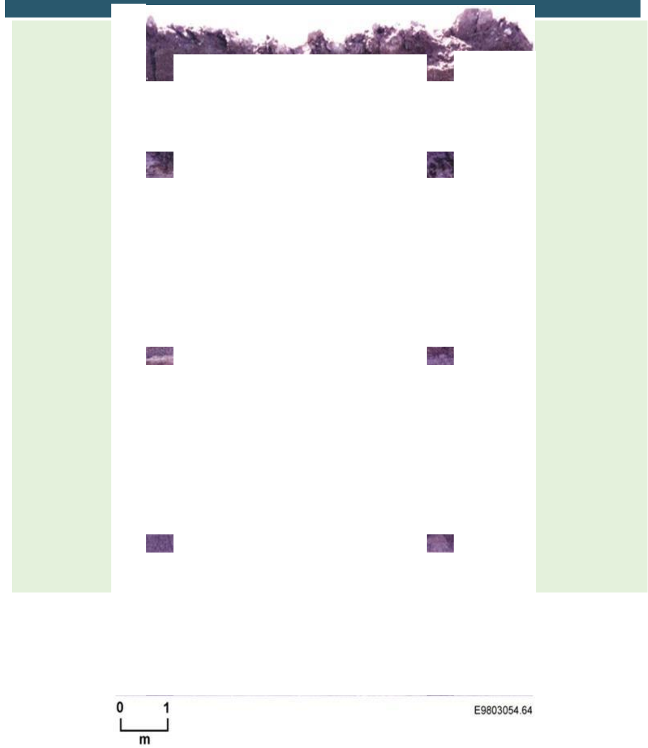
STEP TWO – LUMP OR SPLIT

Use data and site knowledge to refine conceptual model.

Drill cuttings



Split Spoon every 5'



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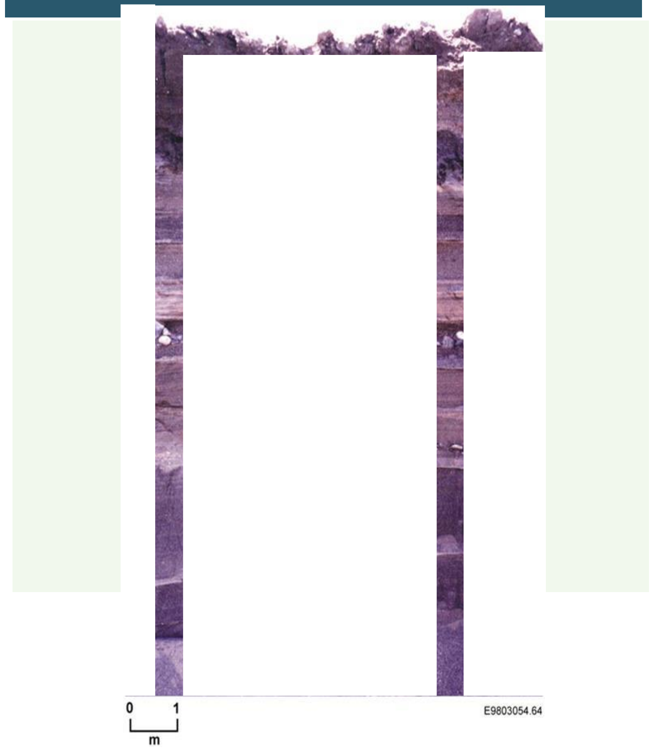

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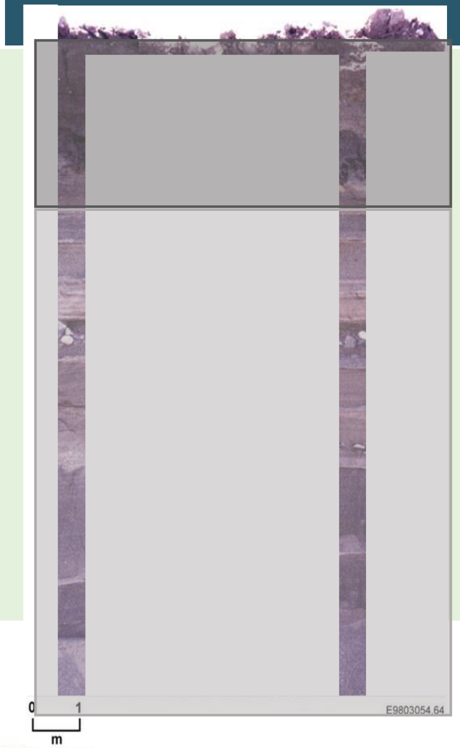
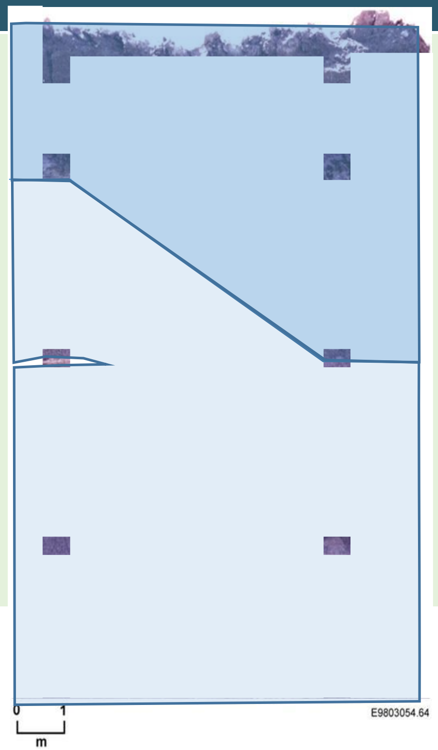
STEP TWO – LUMP OR SPLIT

Drill cuttings



Split Spoon every 5'



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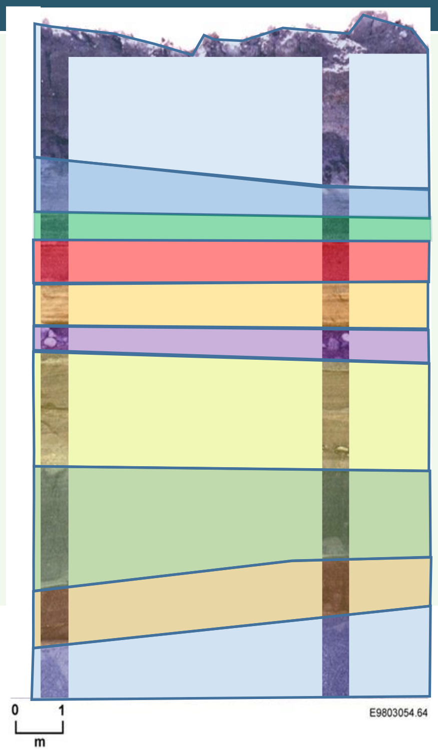

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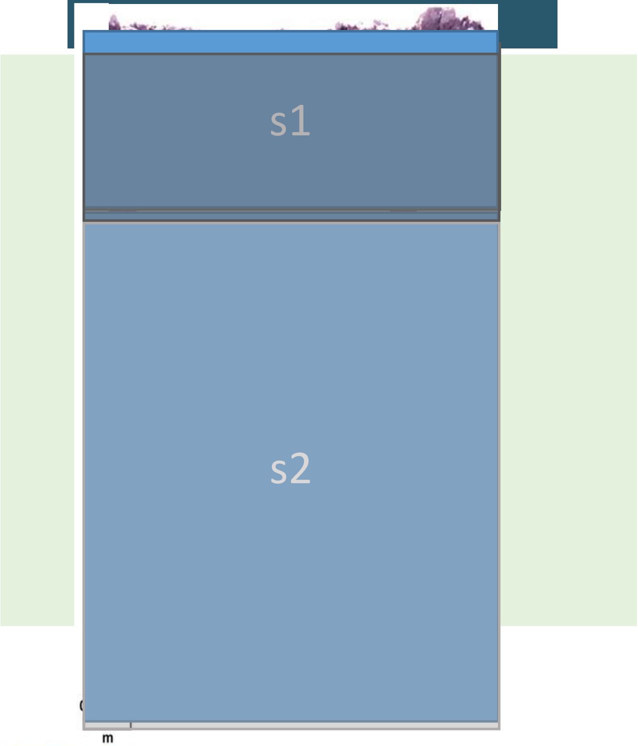
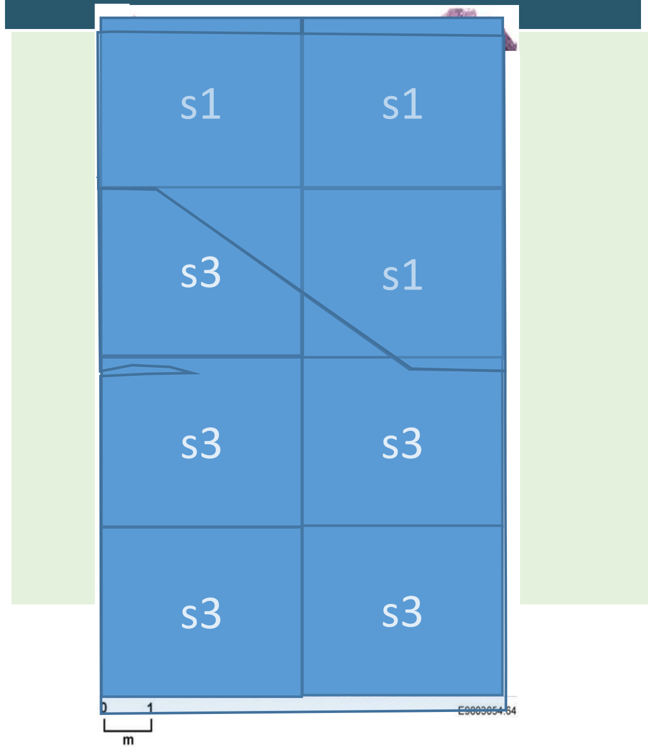
STEP THREE – DISCRETIZE

Make a semi-regular grid of soil types based on cross section.

Drill cuttings



Split Spoon every 5’



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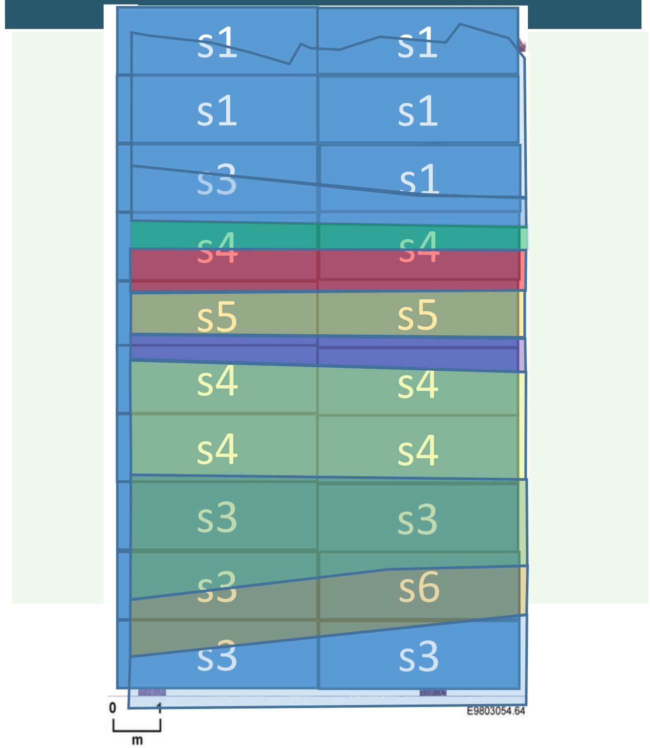

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STEP FOUR – ESTIMATE PARAMETERS

Unit	Description
s1	Fine-medium sand and gravel, trace organic silt/roots
s2	Medium-coarse sand, trace gravel, trace silt (mixed up average from drill cuttings)
s3	Medium sand
s4	Fine sand, some silt
s5	Medium gravel, some coarse sand
s6	Silt and clay

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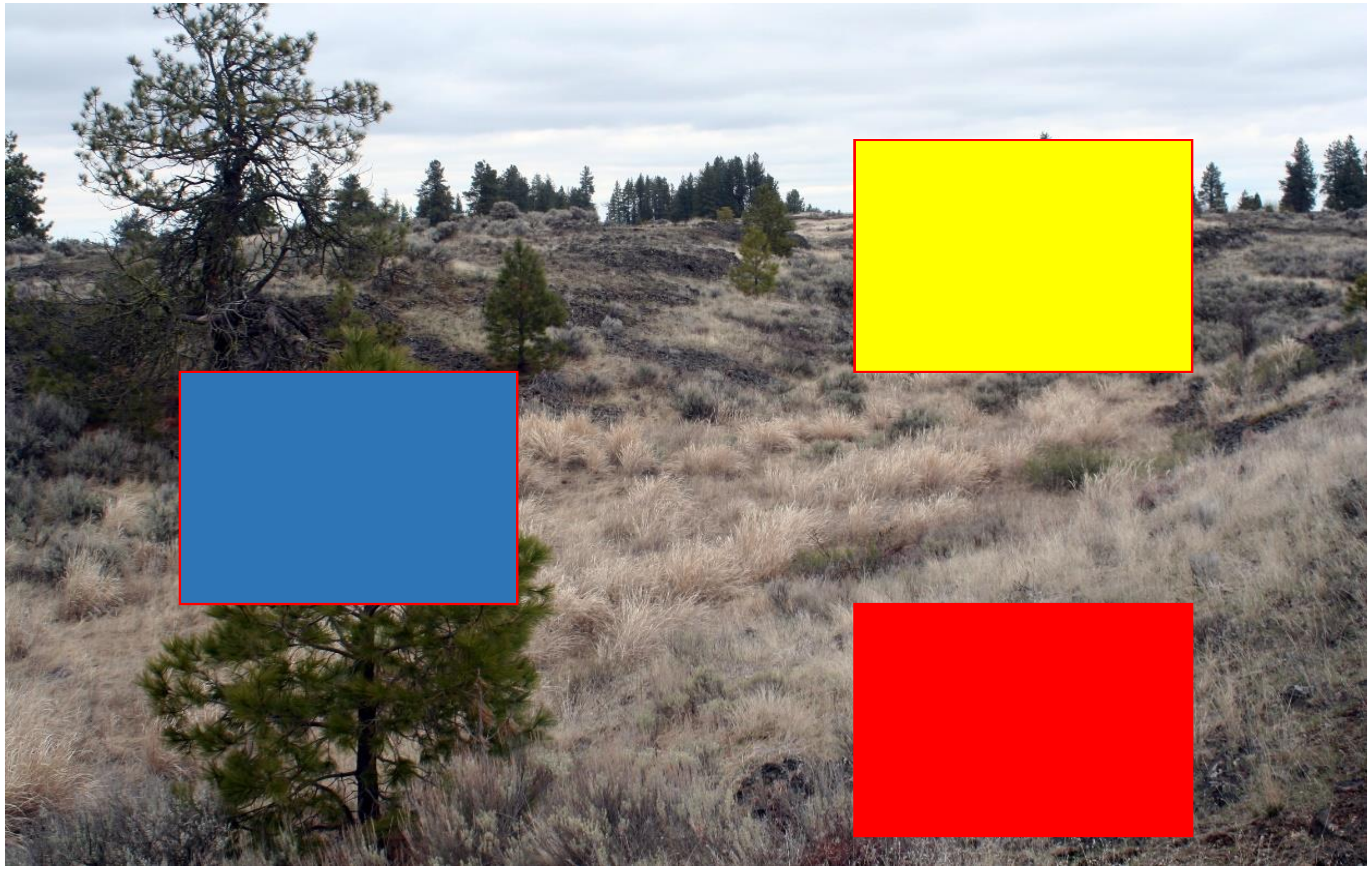
ASSUMPTIONS



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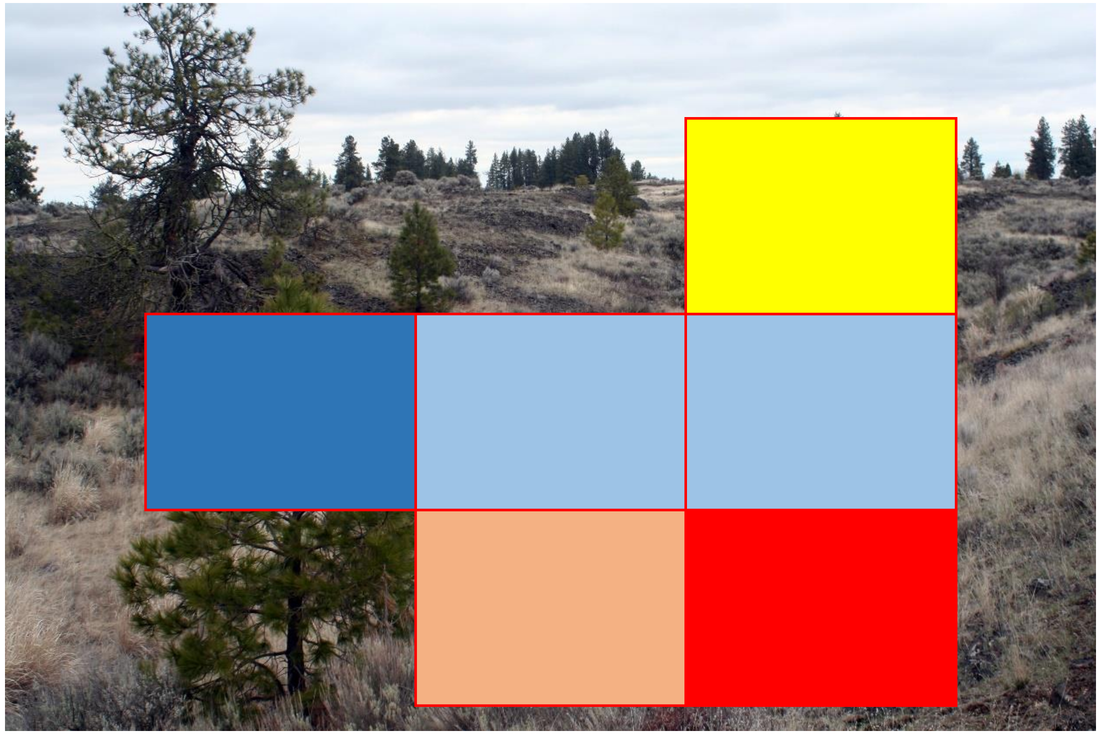
ASSUMPTIONS



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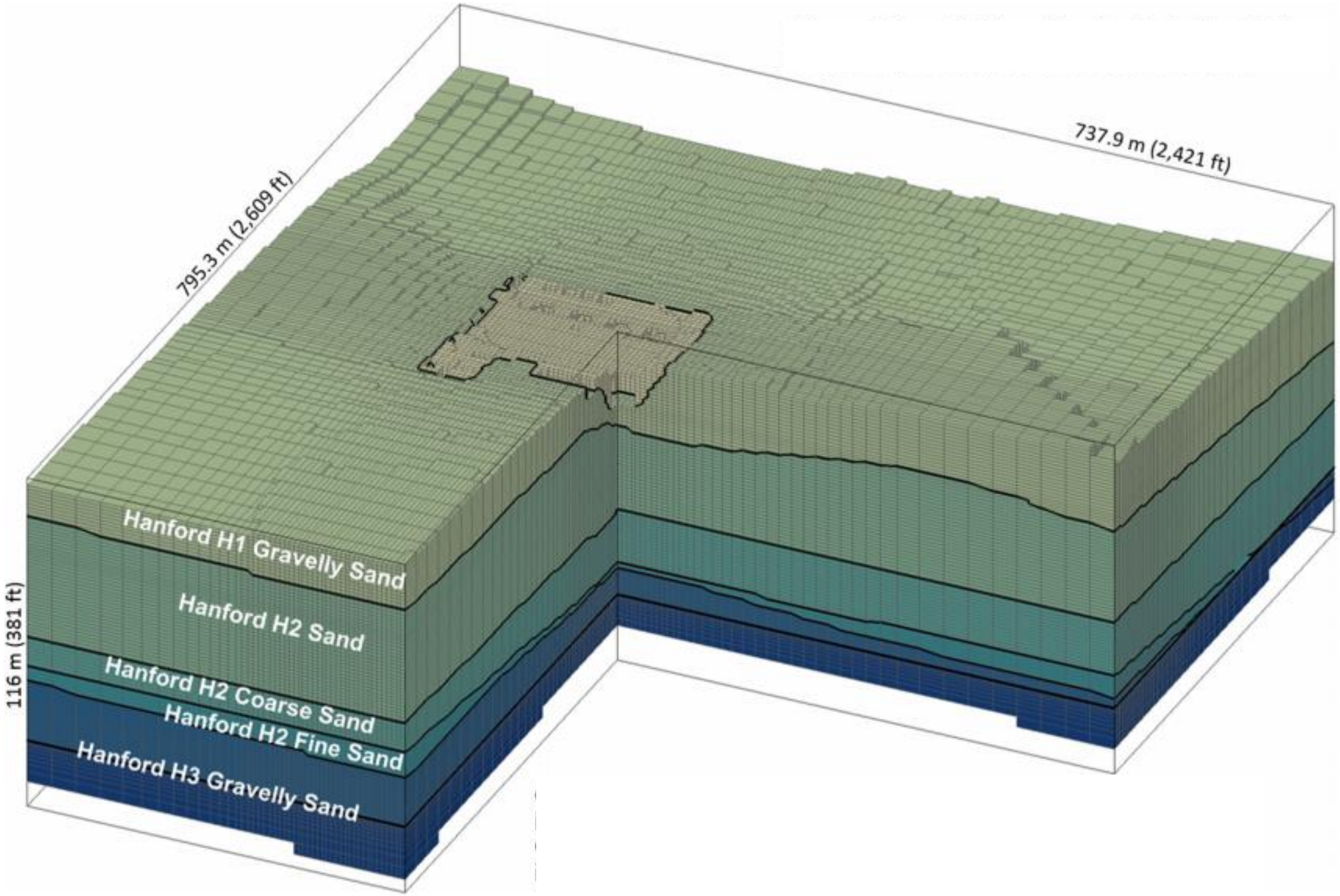
REPEAT AS NEEDED



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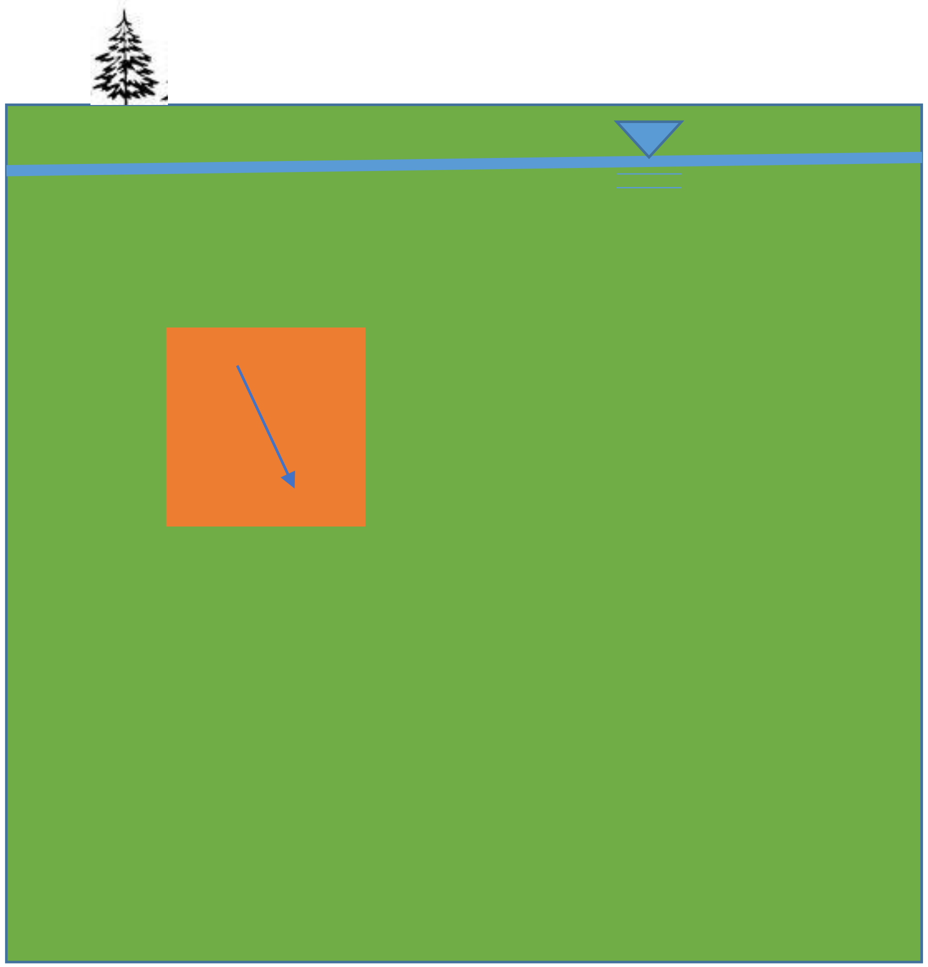
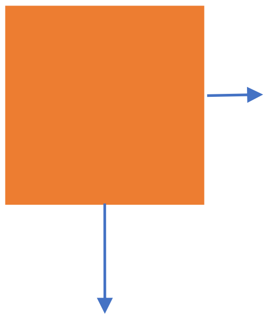
What’s in the box?



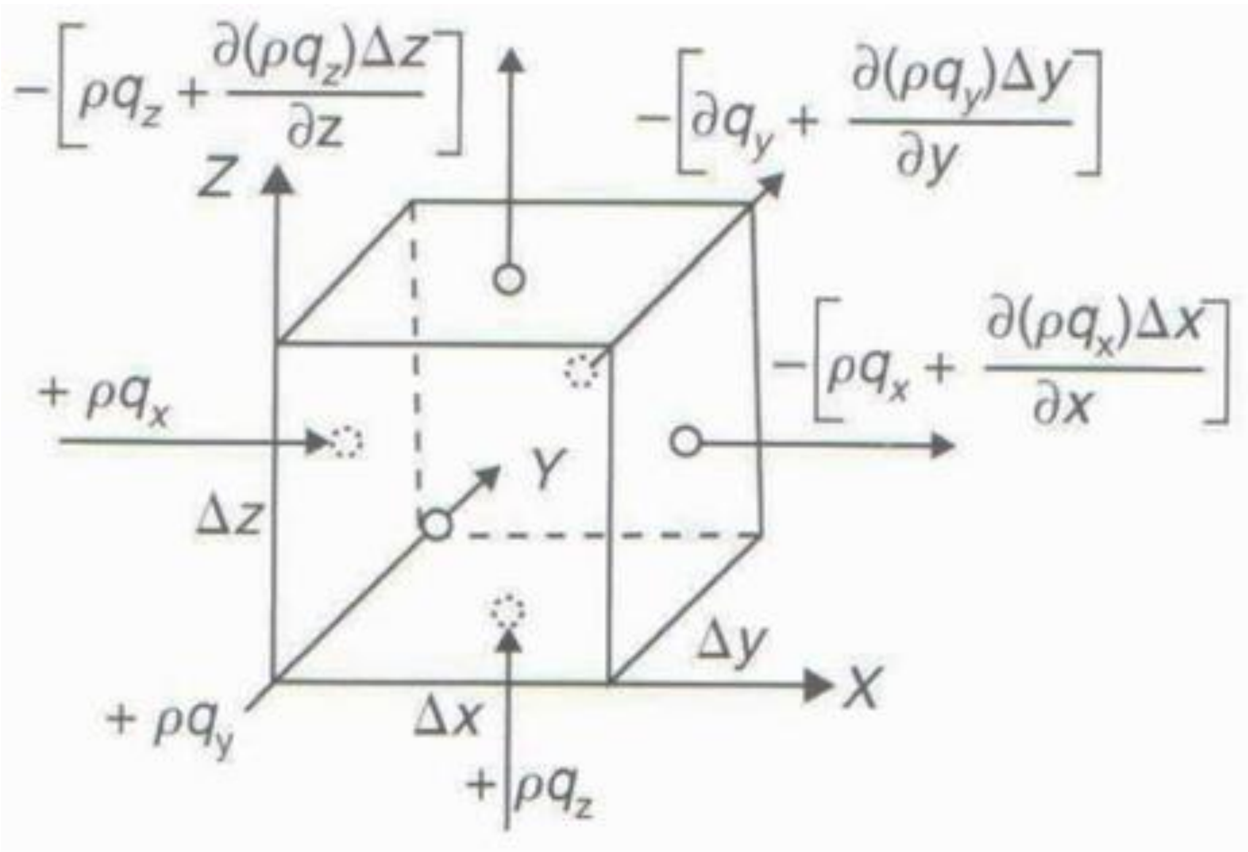
- Contaminated soil
- Some fine layers
- Moving water



PUTTING IT TOGETHER

Sum of the parts

- Software knows what cells are in contact
- In three dimensions, it calculates flow across each plane and travel time across box.
- The flux out of one box goes into the next.



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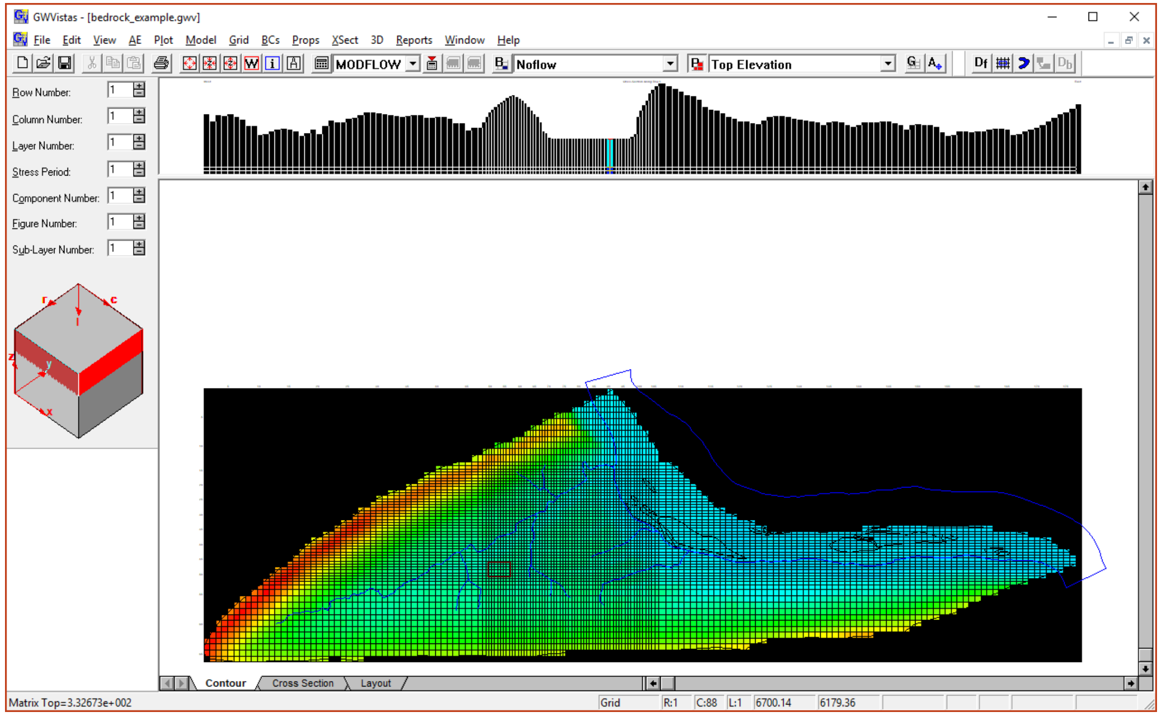
MODEL SPACE AND THE EDGE OF THE WORLD

- What happens when the model runs out of cubes?
- Set a row of "boundary conditions" in each direction
- Constant head, constant flux, no-flow most common



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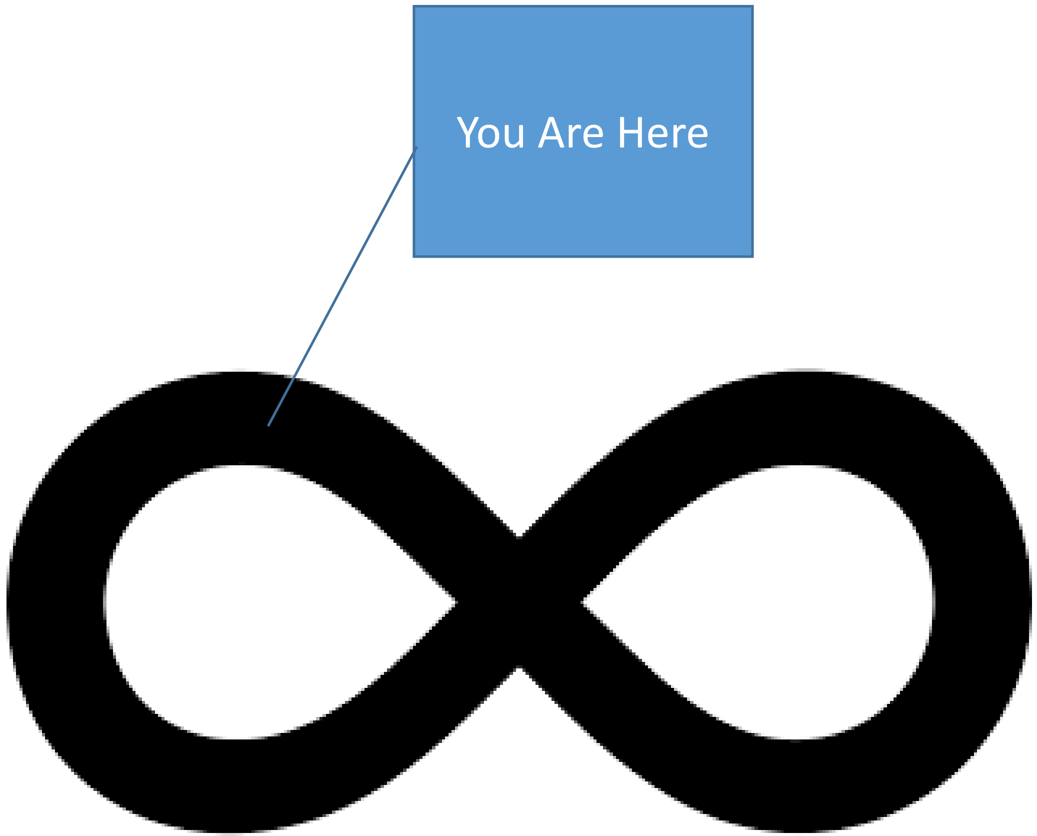


Running the Model

STEP ONE- INITIALIZATION

Fill up the grids and allow background flow to be established

Since model time is quick, this can be run for a couple centuries to make sure everything is in equilibrium.

ONE (A) – FIRST CHECK

If there are wells within the space represented by the model, you can check your boundary condition assumptions by comparing the measured water levels to modeled levels (after initialization)

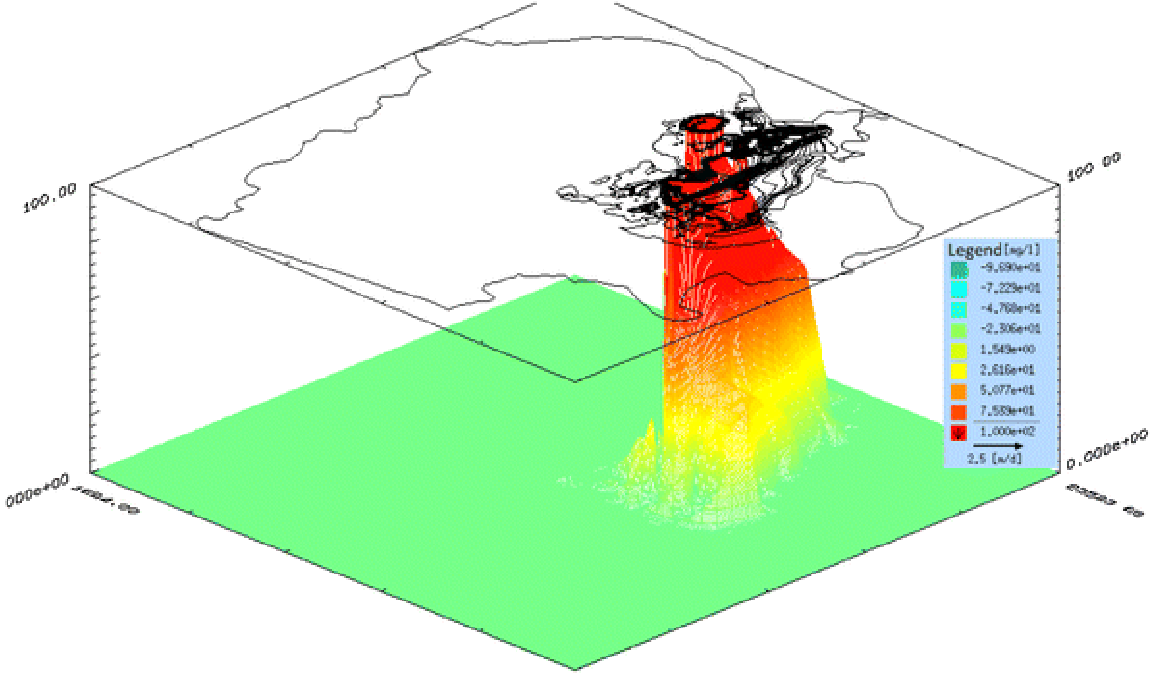
- Revise boundary conditions, re-initialize, and recheck

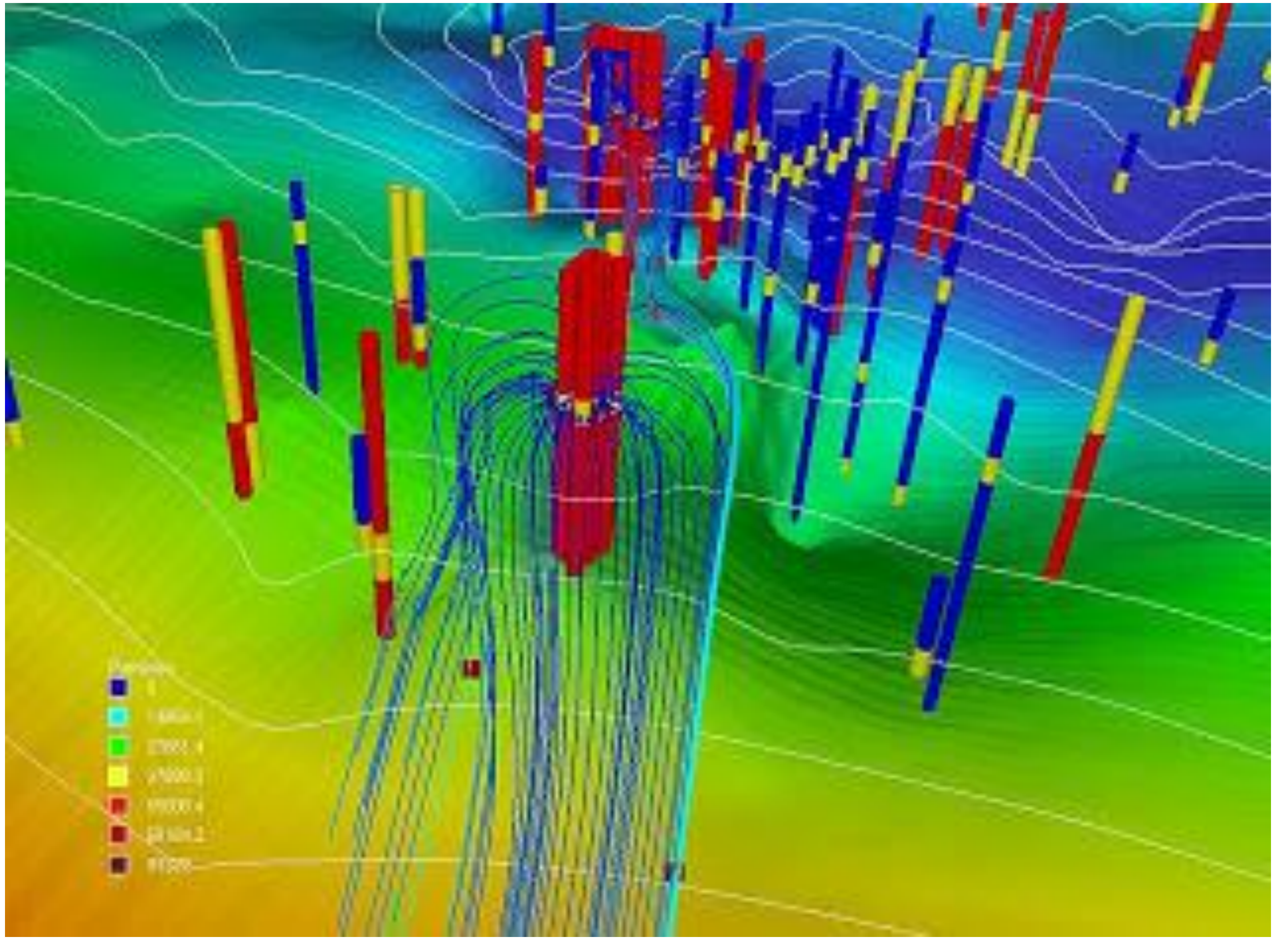
- Proceed to calibration

STEP TWO - CALIBRATE

- Calibration is a systematic adjustment of model parameters to get an expected output with known inputs.
  - Requires field measurements to compare to model output
  - The better the data, the better the calibration – usually a groundwater pumping test with a number of observation wells
  - Hanford “calibrations” use tracers and time (plume flow matching)
- ASTM defines model validation as "the comparison of model results with numerical data independently derived from experiments or observations of the environment.”

STEP THREE – ADD TRACERS AND RUN

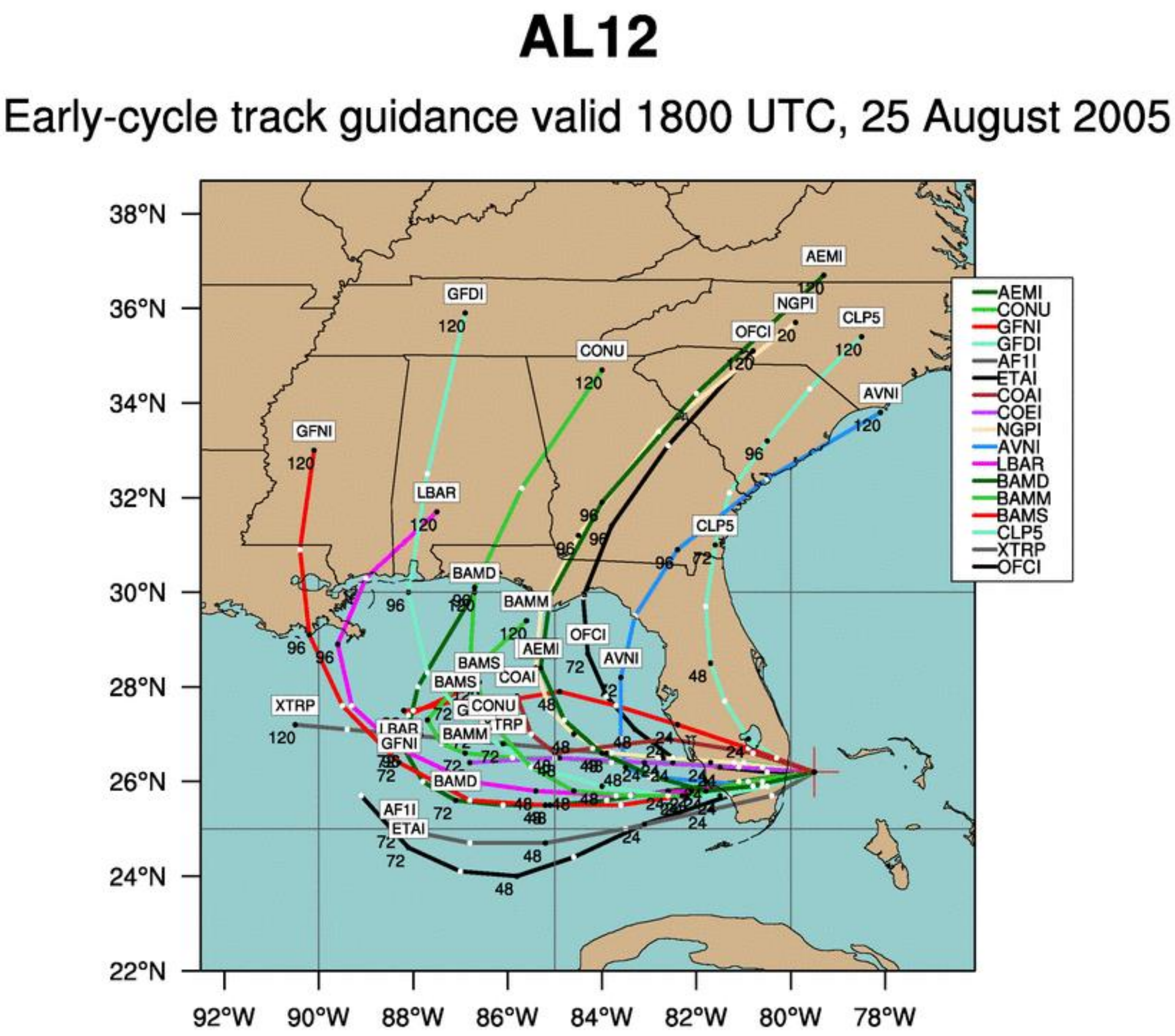




Congratulations! You have a calibrated Deterministic Model!

COMPLEX SYSTEMS HAVE NON-UNIQUE SOLUTIONS

- Depending on the assumptions, you can have multiple calibrated models with drastically different outcomes when you run them forward in time



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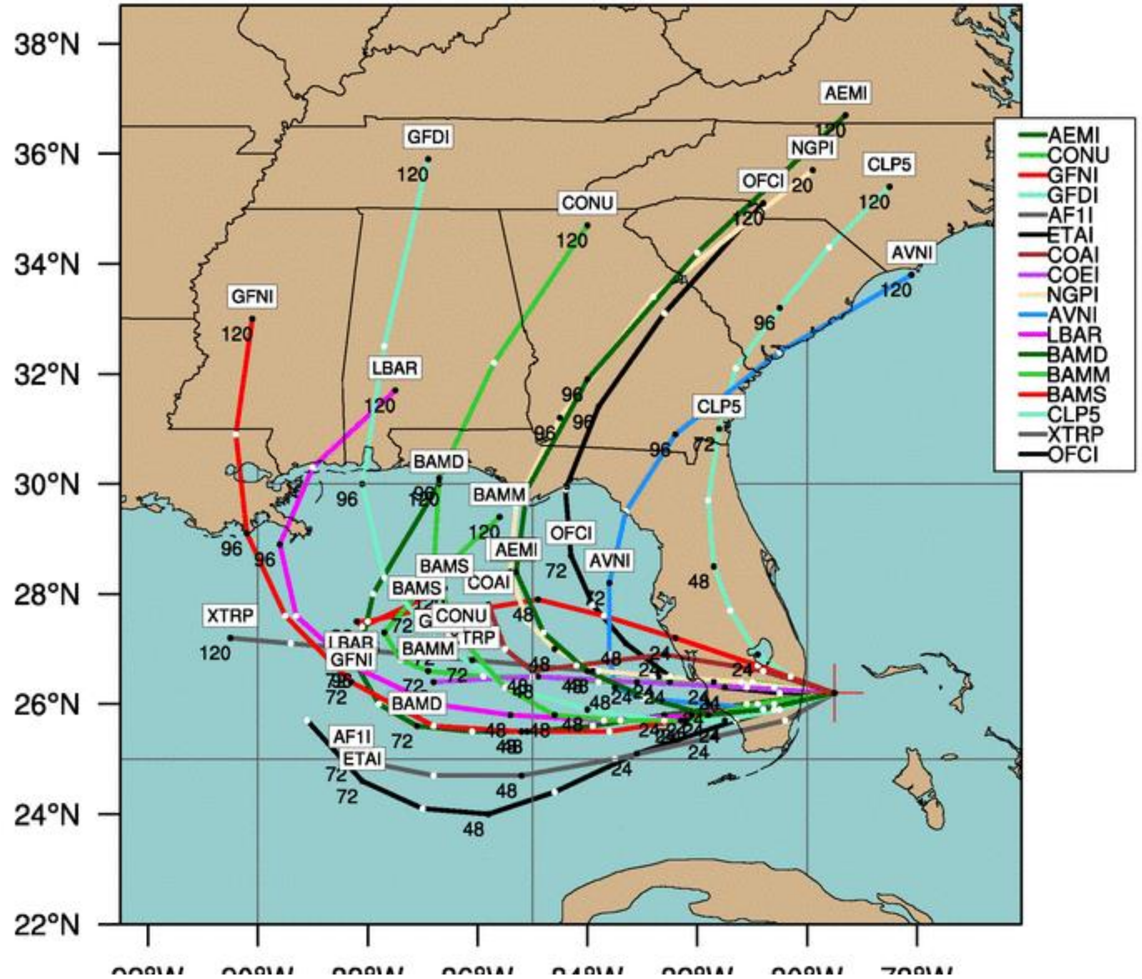
DETERMINISTIC VS PROBABILISTIC

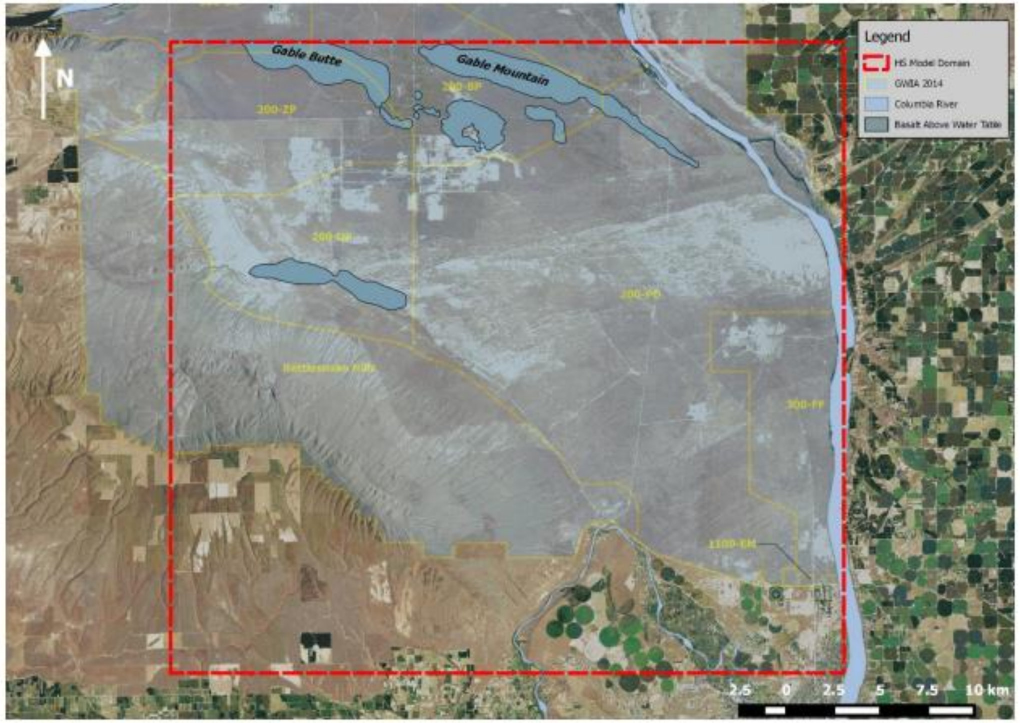
Spaghetti vs the Cone.



HANFORD MODELS

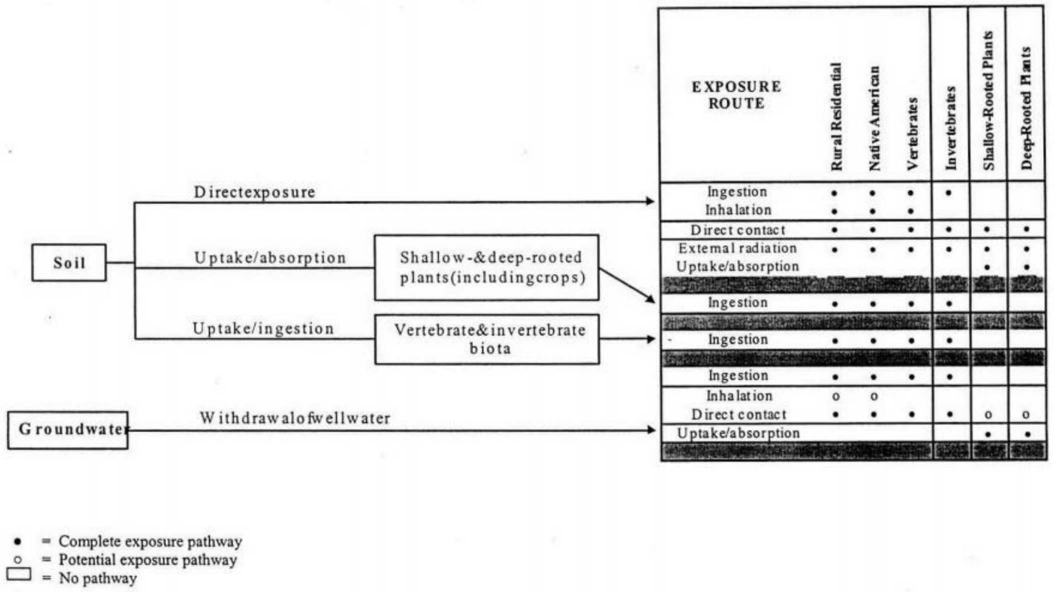
CONCEPTUAL SITE MODELS

Hanford South Geologic Framework Model

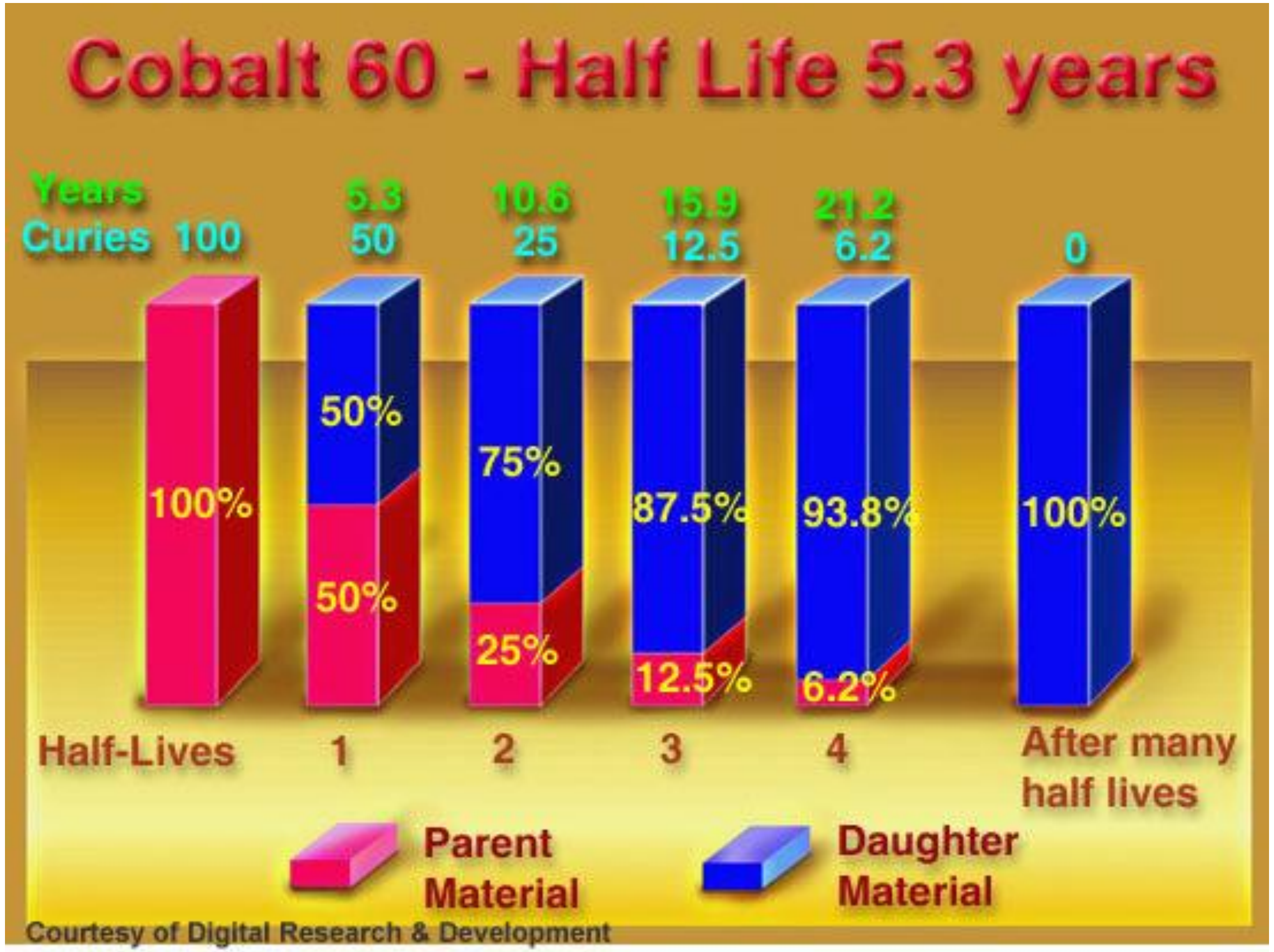


Exposure Pathway Assessment

Figure 5-1. Conceptual Site Model for Upland Zone.



ANALYTICAL MODEL



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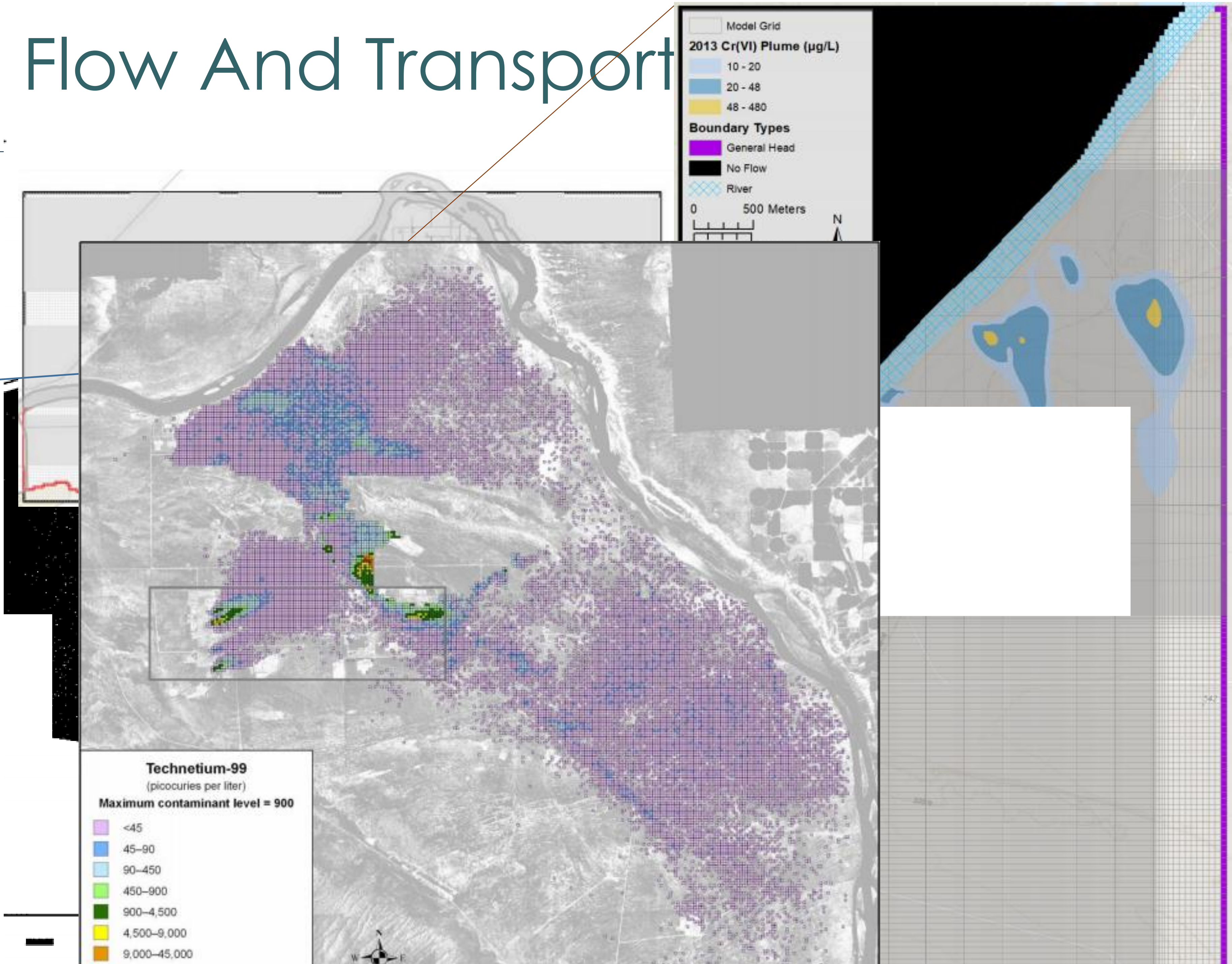
Flow And Transport

Hanford Sitewide Groundwater Flow Model *HSGWF* (2008)



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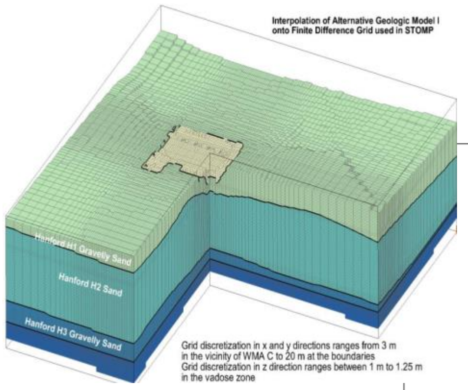
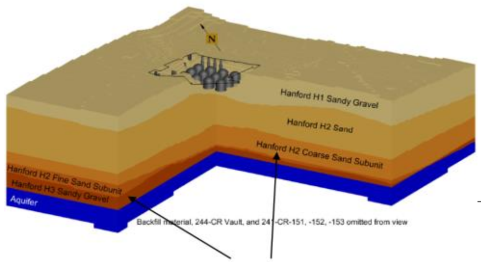
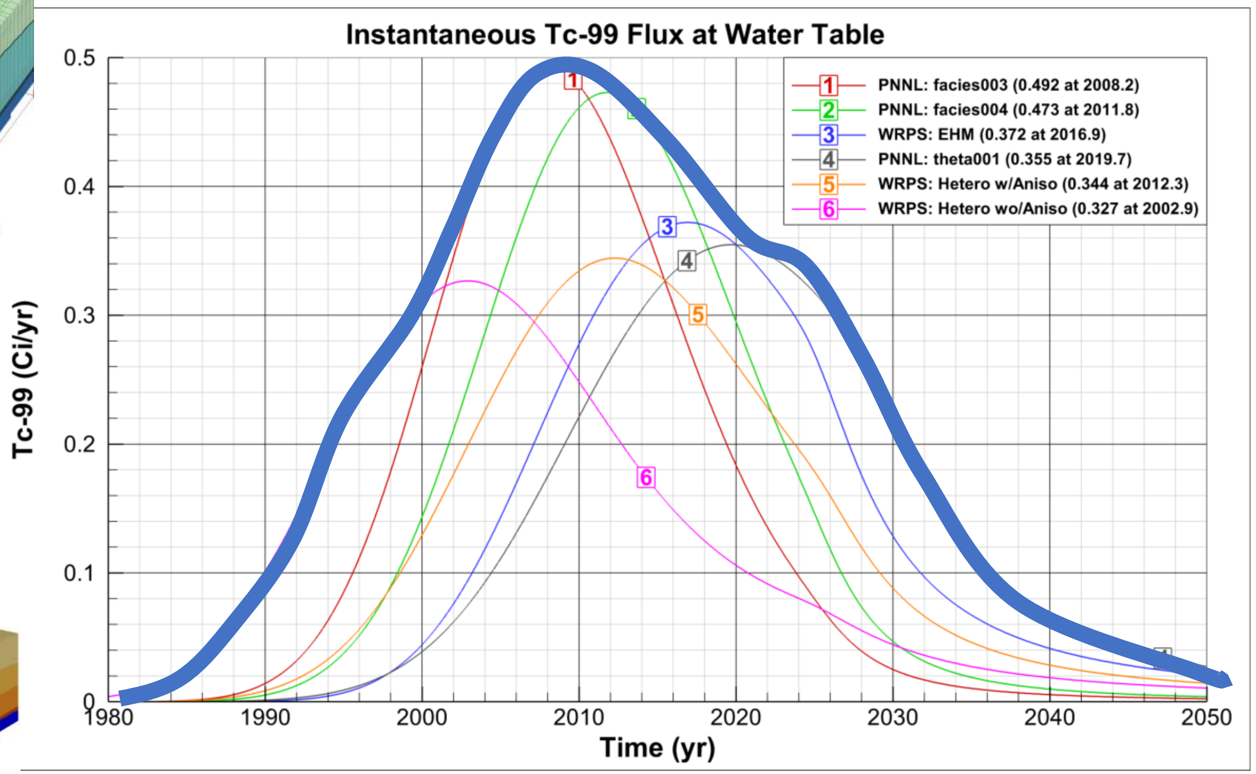
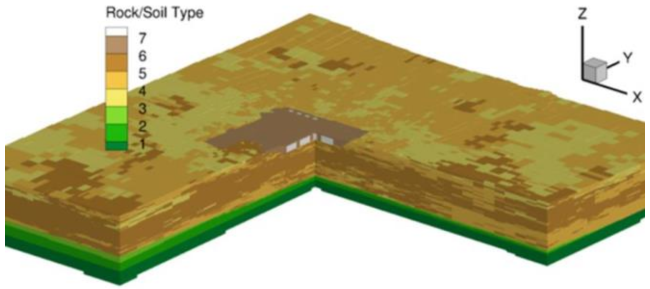
WMA-C - Accidental Cone

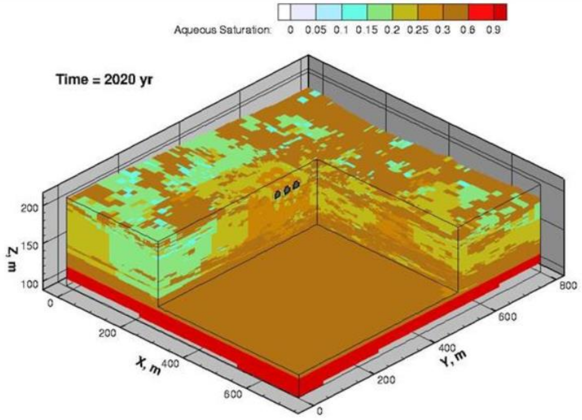


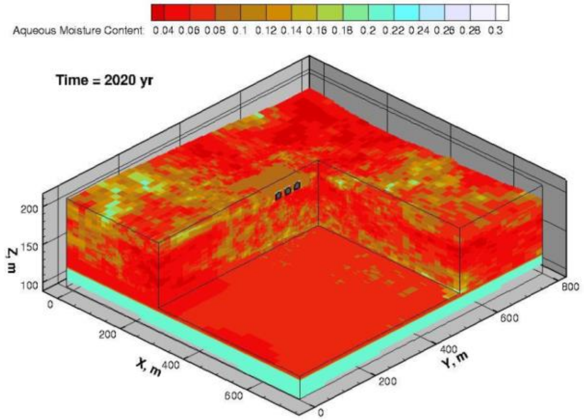


2 additional H2 subfacies

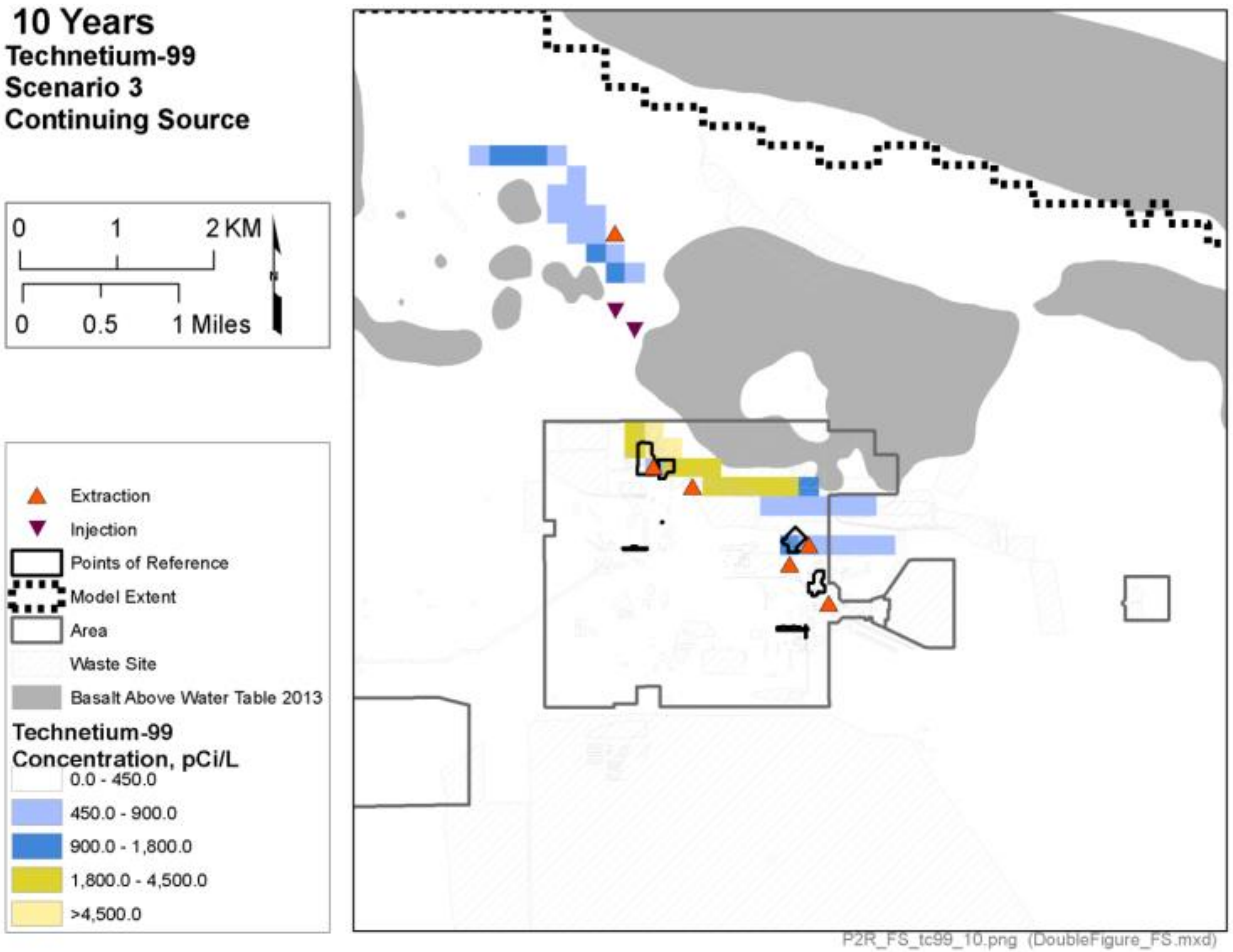








200-BP-5 AND 200-PO-1 P&T FS



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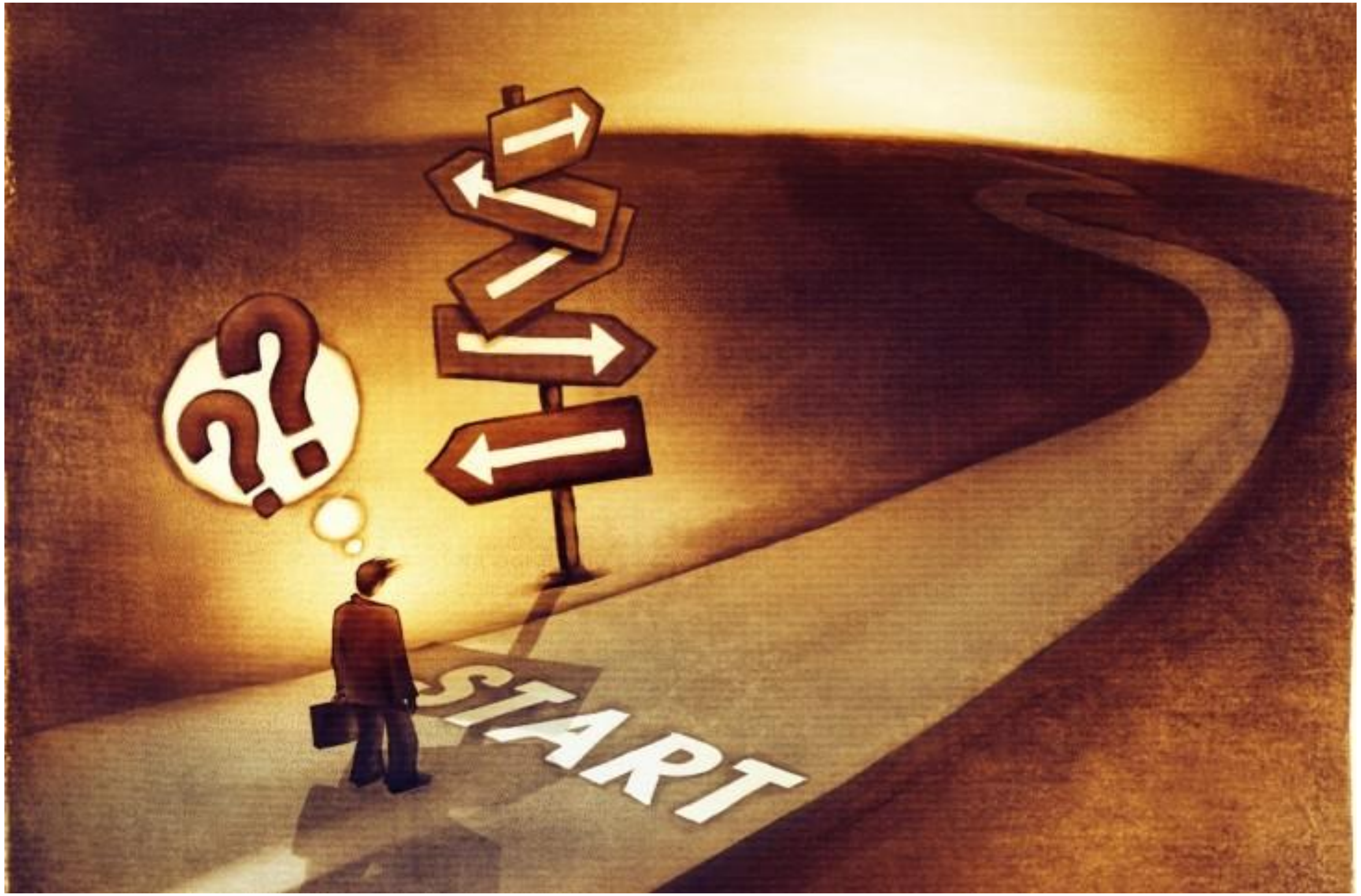
ATMOSPHERIC CALIBRATION

QUESTIONS



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Want to know more?

- https://www.nrdc.org/resources/nontechnical-guide-groundwater-modeling-specific-reference-us-department-energys-hanford
- https://people.maths.ox.ac.uk/erban/Education/StochReacDiff.pdf

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DON'T PRINT_ Extra slides – prob wont use any, just a sandbox

CREATING PROBABILITY DISTRIBTION

- Not all soils are created equal, but variability in natural systems tends to happen in a statistically significant way

- As soil observations and measurements become less, uncertainty increases

- ~~More and more, models are moving to the cone to capture more uncertainty~~

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STOCHASTIC SIMULATION

- Stochastic simulation methods are sophisticated random number generators that allow samples to be drawn from a user-specified target density[4]
- If the parameter in question typically follows a distribution (normal, lognormal, etc.), soil properties are selected at random from that distribution (with some steering data). All of the results within the grid are then averaged.
- If the parameter does not typically fit in a distribution, Monte Carlo simulation is used to select values
- The statistically generated grid is fed into the flow/transport model, and calibrated*.
- The parameters are selected again at "random" and the process is re-run tens to thousands of times.

[4] **A Survey of Stochastic Simulation and Optimization Methods in Signal Processing** Marcelo Pereyra et al, *IEEE Journal of Selected Topics in Signal Processing special issue on Stochastic Simulation and Optimisation in Signal Processing*, March 2016

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* -sometimes

GROUNDWATER MODELS

Refined Grids

1997 Sitewide Groundwater Model

-16 100 Area
dwater Model

2009-17 100 Central Plateau Groundwater Model (version 8.4.5)

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HANFORD MODELS

- Air dispersion models (P&T stacks, PFP demolition, Tank farm stacks)
  - Used to document compliance with WA air regs and evaluate exclusion areas for demolition
  - https://pdw.hanford.gov/arpir/pdf.cfm?accession=D196068325

- Hanford Site Groundwater Flow Model (HSGW Model)
- Waiting on Revision 1
- 100-Area Groundwater Fate and Transport Model (100AGWM)
- https://pdw.hanford.gov/arpir/pdf.cfm?accession=0076173H
  - https://pdw.hanford.gov/arpir/pdf.cfm?accession=0087245
  - Grid is 100 m, fines to 15m in OUs
  - 100-NR-2 Scale-Appropriate Fate and Transport (100NSFT) Model
    - https://pdw.hanford.gov/arpir/pdf.cfm?accession=0064806H
    - Grid is 2.5-15 meters
- https://www.hanford.gov/files.cfm/Attachment%204_GW%20Models.pdf

- Stream tubes
- https://www.hanford.gov/files.cfm/DOE_EIS-0391_2012_App%20O%20Groundwater%20Transport%20Analysis.pdf

- Plateau to River Groundwater Transport Model (P2R Model)
- https://pdw.hanford.gov/arpir/pdf.cfm?accession=0080149H
- Piecemeal while waiting on HSGW rev

- Central Plateau Groundwater Model (CPGW Model)
  - - https://pdw.hanford.gov/arpir/pdf.cfm?accession=0066449H
  - 100 m grid
- 300 area with stochastic
- https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-17708.pdf
- Hanford South Geologic Framework Model (GFM)

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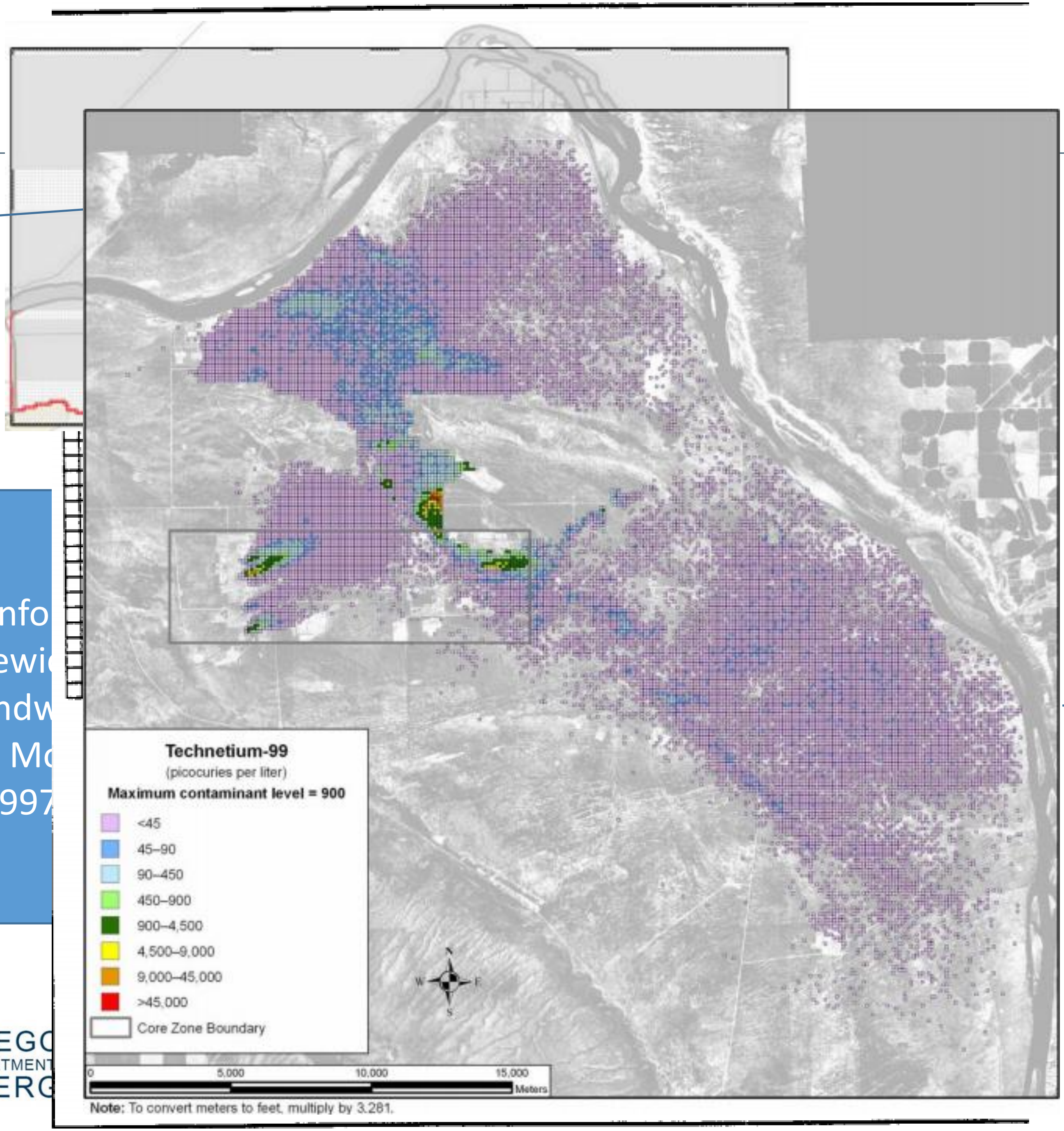

Hanford Sitewide Groundwater Flow Model *HSGWF* (2008) – revision due

Plateau To River Model *P2R* (2015)

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- Other slides
  - How to populate unknown grids
    - Cammo
    - Kriging
    - Linear
    - Nearest neighbor
    - Statistics

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LOSE LOGO IF PIC OR GRAHPIC IS TOO BIG