Basic Settings for Building a Better Model

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CLU-IN webinar in December, 2019

Outline

- Important issues for setting up a groundwater model
- Basic checks for a flow and transport model
- Uncertainty analysis
- A modeling framework may be useful

Before Modeling

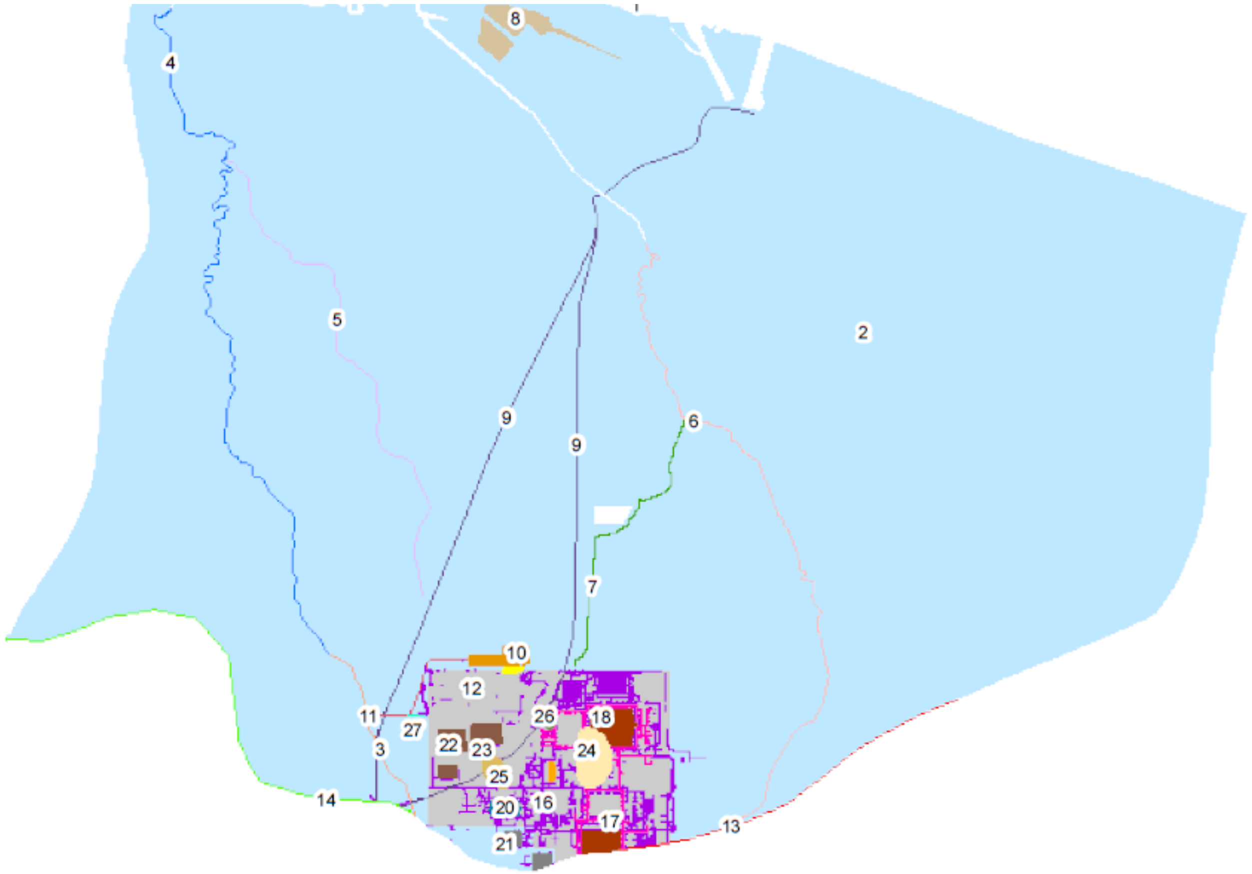
- CSM (conceptual site model)
- Plan view (DEM) of the model domain
- X-section (lithology)
- Physical and Hydrogeologic conditions (e.g., porous system or fractured rock)
- Modeling objectives
- Data availability/Data gaps?
- Is modeling necessary to get an answer for decision making?

Initial Preparation for Groundwater Modeling

- What datasets represent the best steady-state flow condition?
  - Separate datasets for **calibration** and **validation**
- Are there any datasets for transient flow calibration?
- Identify the Target wells
- Is the source mass/concentration decaying?
- What is a reasonable estimate for partitioning coefficient (i.e., retardation factor)
- Is biodegradation happening? Do you degradation products? Any approximation of the biodegradation rate?
- Is the selected modeling package robust enough to handle the geochemical processes?

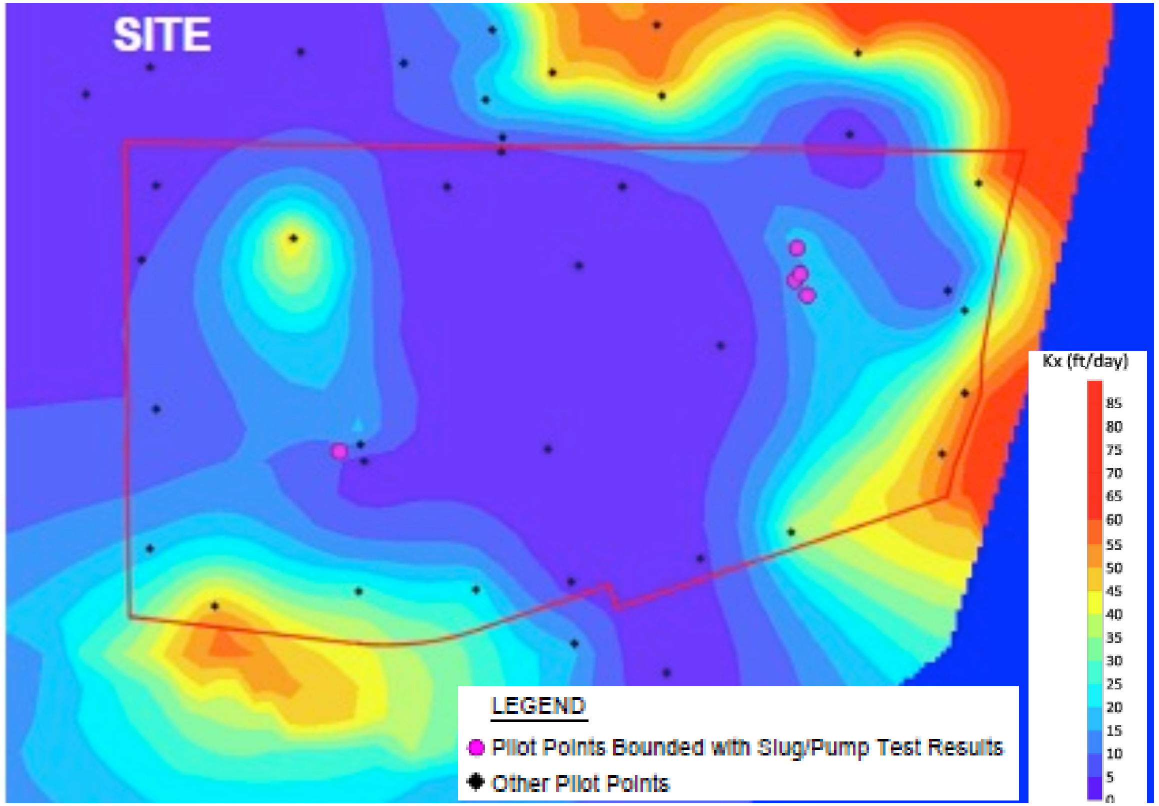
Model Setup

- Large enough model domain.
- Lithology well represented in the model layers?
- Boundary Conditions well understood;
  - Find a set of target wells near the boundaries to validate the boundary values
  - Do not set up ‘Constant Head Boundary’ near an extraction well
- Calibration Targets: Do not average the elevation data, instead use a given sampling dataset (snapshot)



Flow Model Calibration

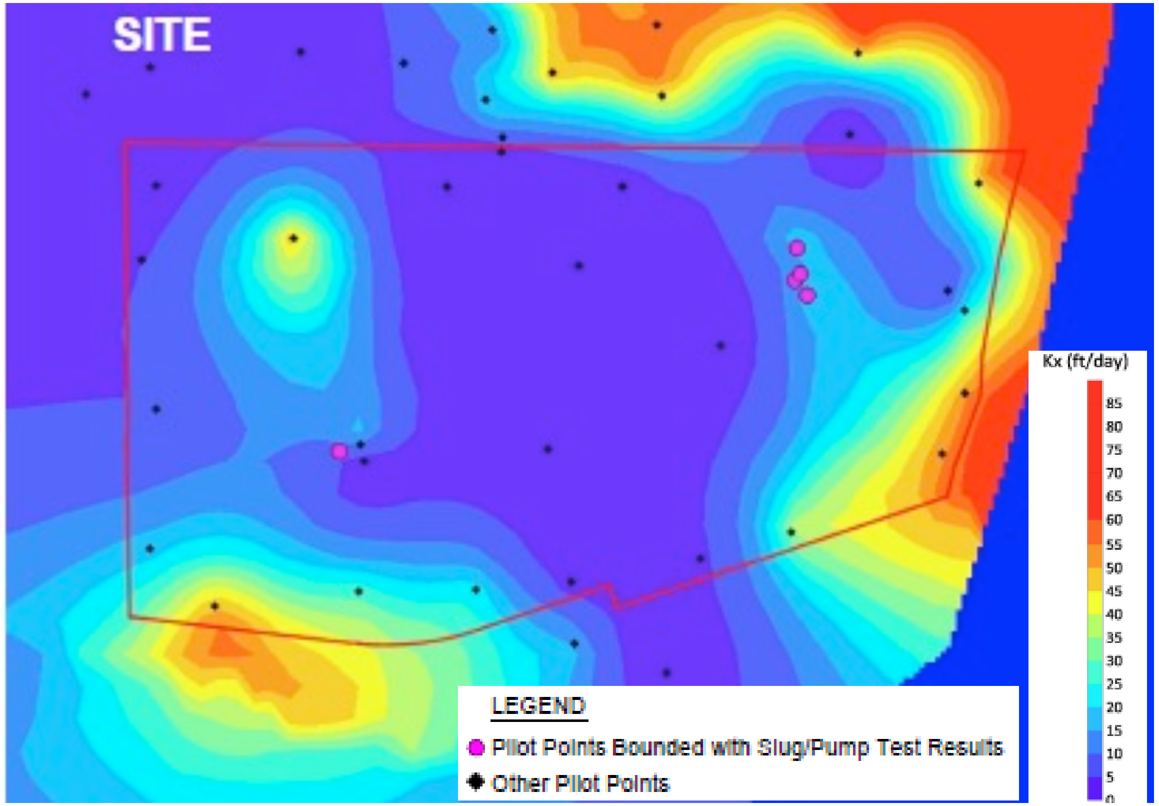
- More data is available for flow model calibration
- Transport model depends on the flow model
- **Manual vs. Automated (PEST) calibration?**
- PEST is inverse modeling tool for automated calibration of model parameters.
- PEST is popular among modelers/consultants
- Pilot Points in PEST should be limited in numbers and have a tight range for each parameter
- Initial values are sensitive in PEST calibration
- <u>Start with manual calibration and then improve with PEST</u> – *Rarely/Never followed in practice*!!



Calibrated hydraulic conductivity of surficial aquifer

Flow Model Calibration (contd.)

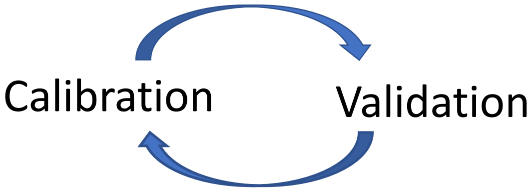
- Calibration criteria in industry is NRMSE <= 10%
- NRMSE (Normalized Root Mean Square of Error)
- NRMSE = RMSE/(Range of Observed Head) ×100%
- **Goal** should be **NRMSE≈5% in the key areas/layers**
  - Group target wells for calibration in the key areas
  - Try to achieve NRMSE≈5% in the key areas
  - Do not just check site-wide NRMSE <=10%
- Also qualitatively match observed vs. calibrated potentiometric surface maps.



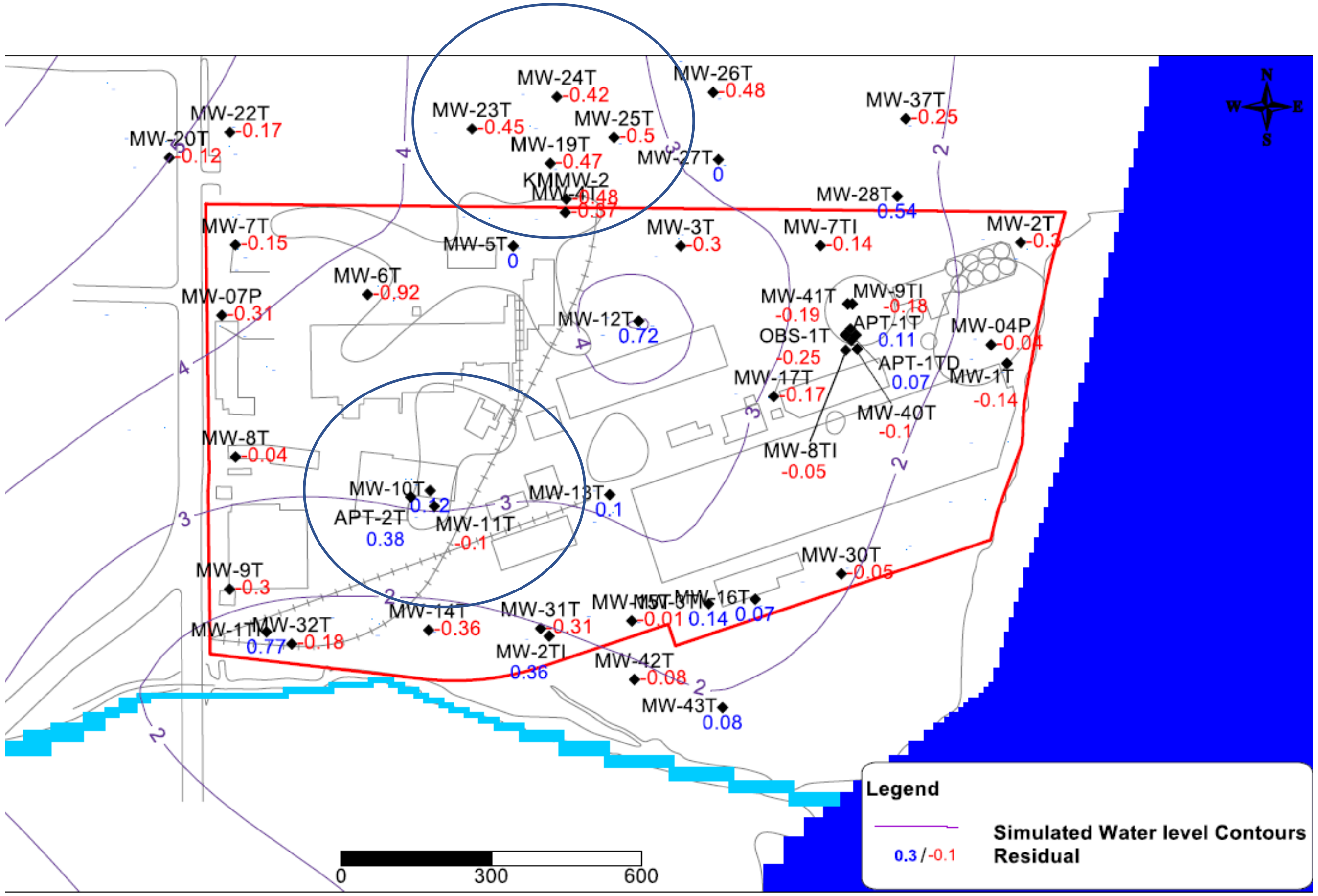
Calibrated hydraulic conductivity of surficial aquifer

Calibration/Validation

- Residual Distribution Map
  - ❖ Residual Error should be well distributed
  - ❖ Avoid bias to minimize error in hydraulic gradient
- Validation should be done with a dataset not used in calibration
- Calibration-Validation is an iterative process



- Validation is not popular among consultants!



Sensitivity/Uncertainty Analysis

- Parameter sensitivity is most commonly done in practice
- Again, not so popular among consultants!
- Common practice is to **compare the RMSE values between simulated and the calibrated models**.
    - ❖Doesn't help in decision making, since it doesn't address sensitivity to the model objectives. For example ,
        - ❑Capture zones in a pump & treat system
        - ❑Time to reach the cleanup goal
- We expect to see model uncertainty as it relates to the modeling objectives and identify data gaps to address that uncertainty.

Solute Transport Model

- ❑ Three common questionable practices
  - ❖ Retardation Factor (RF) is too high!
  - ❖ Source is instantaneous/initial?
  - ❖ Biodegradation Rate (half-life) calibration?

❖ RF could be estimated in the following ways,

1. Find the partitioning coefficient (K_d) from batch or column test
2. Measure fraction of organic carbon (f_{OC}) from the site soil and use literature to get K_{OC} for each COC. (*most commonly done*)
3. Calibrate in the solute transport model

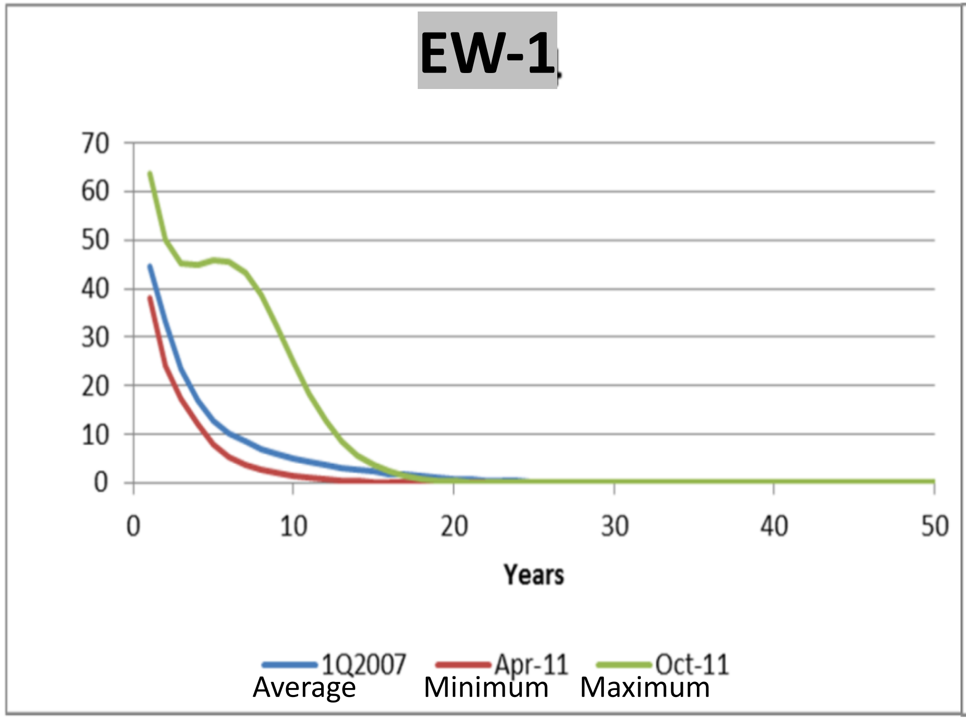
- ➢ Batch test will usually generate high values of K_d (i.e., high RF),
- ➢ f_{OC} from the contaminated subsurface soil sample will be very high and thus result in high RF (*very common mistake*). Need to test on background samples.
- ➢ Initial estimation from column test of undisturbed soil sample followed by model calibration is likely the best option (time consuming and costly)
- ➢ Calibration of RF has high uncertainty, because of too many sensitive model parameters.

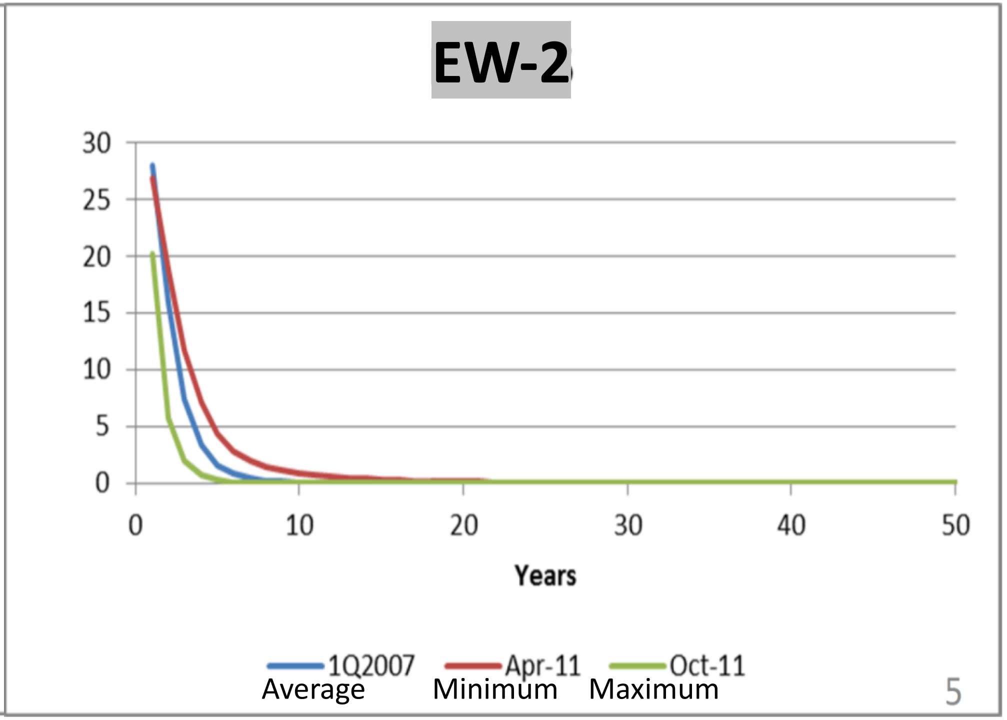
❑ Particle tracking modeling shows groundwater flow direction (Need a good flow model).

Solute Transport/Instantaneous Source

- Initial concentration of the plume is assigned, but no continuous source!?
- Plume in the source area will deplete quickly unless the K_d is very high (Figure)
- Artificially high K_d is sometime used to model back diffusion. (questionable practice!)

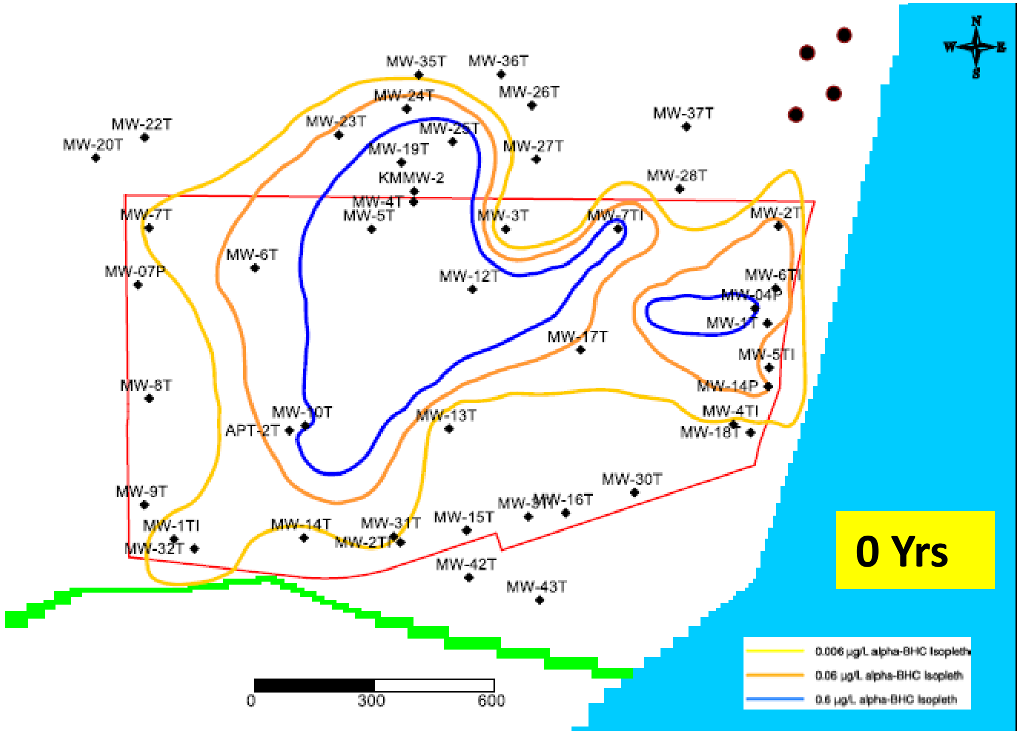
❑Historic matching of the source concentration must be done to define the source boundary in the model.

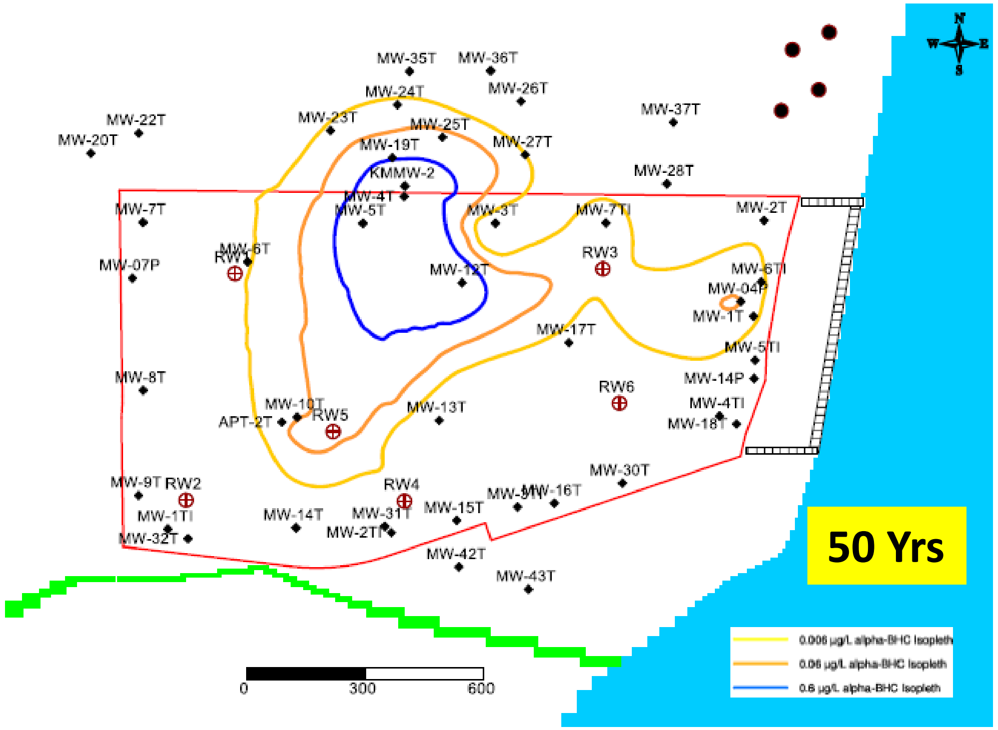




Solute Transport/Biodegradation Rate

- Do a well-by-well trend analysis and estimate the decay rate (k).
- Biodegradation rate (ϒ) is NOT k. (Ideally, ϒ<<k)
- Look for daughter products to confirm biodegradation is happening!
- Biodegradation rate is usually not uniform throughout the site.





Half-Life = 13 yrs (from calibration); i.e., 1 order of magnitude concentration decrease in about 40 yrs.

Solution?

- Get involved early, not after the consultant has completed his calibration and used up all the funding (*often the case*).
- Make sure to discuss the modeling framework and workplan in the beginning?
- Specific modeling guideline is not available (to my knowledge).
- Modeling world is vast and it’s hard to cover every aspect through a guideline
- Wanted to highlight some common issues rather than trying to cover the broad spectrum in the modeling world!
- A simple modeling framework/checklist might be needed!

Thank You
Question and Comments