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# Estimating parameters and uncertainty for three-dimensional flow and transport in a highly heterogeneous sand box experiment

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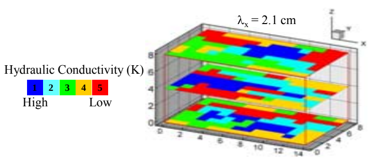
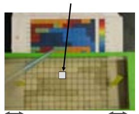
## Objective

- Tracer concentration breakthrough curves (BTCs) obtained from a magnetic resonance imaging (MRI) technique in a small 3D flow cell were used to
  - evaluate inverse parameter estimation techniques with different approaches to parameterization of the spatial fields (e.g., hydraulic conductivity, porosity, and dispersion coefficients)
  - identify the data worth for transport problems

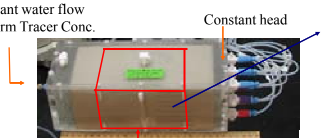
## Laboratory-Scale Experimental Setup

- Sand distribution generated using SISIM in GSLIB
  - 14 x 8 x 8 $cm^3$, 1 $cm^3$ grid (896 cells) with 5 different size of sands (~20% each)

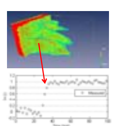



- Constructed a heterogeneous permeability field in a 3D flowcell (21 x 9 x 8.5 $cm^3$) and purged with a solution of tracer uniformly
  - Permeability, porosity, longitudinal dispersivity values for each sand type were independently measured
  - Measured tracer signal using MRI at a voxel scale (~0.1875x0.1875x0.225 $cm^3$) at a regular interval (130 s) time over 4 hrs → converted to concentrations (BTCs)




Heterogeneous region for MR Imaging : 13 x 8 x 8 $cm^3$

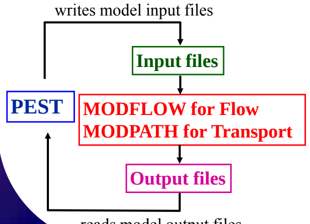


Paramagnetic tracer imaged by MRI scans (Yoon et al., 2008)

## Inverse Modeling

- Numerical domain: 21 x 8.8 x 8.5 $cm^3$ (numerical grid of 0.25 cm)
- Observed data for inverse modeling:
  Mean arrival times of tracer at two different scales (0.25 cm and 1 cm)
- Model parameters for estimation: hydraulic conductivity and porosity
- Pilot Points: vary properties using a kriging method
- Measurement errors in different sand types (i.e., weighting factors)
- Different prior information (e.g., zonal information) will be tested against the case of more pilot points

### PEST (Parameter ESTimation Software)




- PEST: Model-independent calibration tool

♦ Parameter Estimation: Calculates sensitivities between model output and groups of specific model parameters

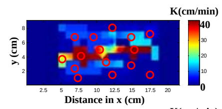
♦ Predictive Uncertainty: Determines how uncertainty in input parameters affects specific model output

♦ Singular Value Decomposition Analysis with highly parameterized inversion

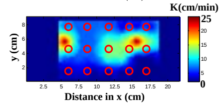
## Modeling Variablility

- Aquifer properties (e.g., permeability, porosity) are spatially variable
- Pilot Point method: Property values are assigned to a set of pilot points distributed through the model domain
- Property values in the rest of the domain are assigned through spatial interpolation (i.e., ordinary kriging method) from the pilot points, which was used for each physical layer (4 vertical numerical grid)

♦ Coupled Zonation and Pilot-Point approach with less number of parameters

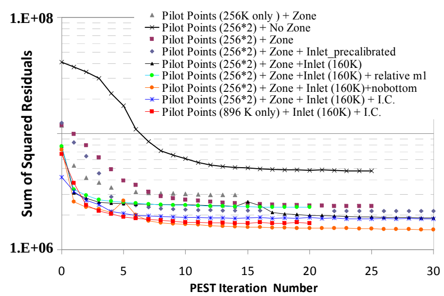



♦ Pilot-Point approach with high number of parameters




## Parameter Estimation

- Objective function for inverse modeling: Sum of squared differences between measured and modeled mean arrival times (m1) at 0.25 x 0.25 x 0.25 $cm^3$

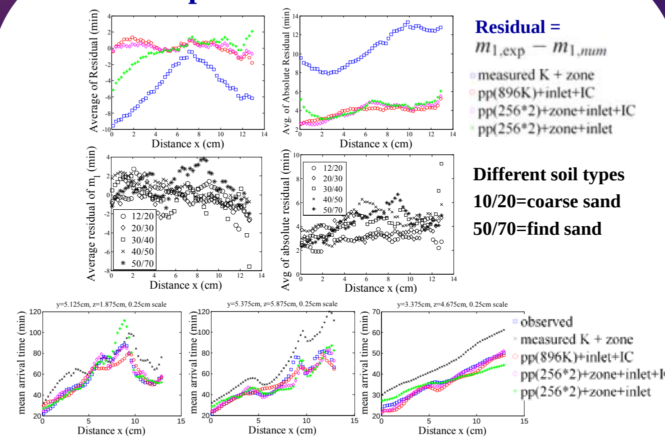



**Pilot Points (256*2):** 256 pilot points for both K and porosity (~32 points per each layer)
**Inlet_precalibrated**: K in the inlet region was calibrated independently
**Relative m1:** observed m1/simulated m1 as observation data
**no bottom:** data on the bottom 0.25 cm was not included due to its poor data quality
**I.C.**: tracer is initially located in the inlet region by 1cm, otherwise, no tracer in the domain

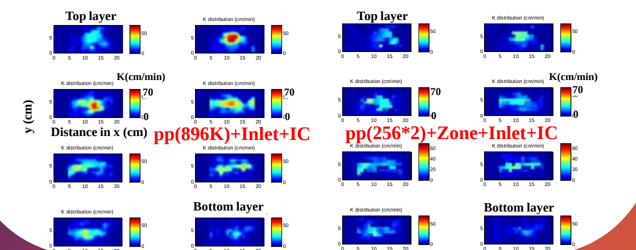
### Summary

- Zone: The detailed zone information was used as prior information to constrain the spatial impact of the pilot points and reduce the number of parameters
- Porosity: Porosity was very sensitive to mean arrival times, so porosity values were bounded between 0.31 and 0.37 based on measured porosity distribution. Inclusion of porosity did not reduce the objective function much, however, estimated K distributions with porosity as a parameter have lower range, compared to highly parameterized case (pp(896K only)+Inlet+IC)
- No bottom : Exclusion of observation data on the bottom 0.25 cm (~ 3% of total data) improved the objective function by 19%.
- I.C.: Inclusion of initial condition improved estimation of m1 in the inlet of heterogeneous region
- Preliminary results with BTCs at 1 cm scale show that objective function can be < 5000, indicating higher objective function at 0.25 cm scale can be attributed to local scale heterogeneity

## Comparison of mean arrival time




## Estimated K distribution




## SUMMARY & FUTURE WORK

- Two approaches including the detailed zone information with less pilot points and highly parameterized inversion with pilot points are compatible, but the range of K distribution was different, which may be attributed to the effect of porosity.
- Data quality (e.g., measurement error), measurement scales (e.g., 0.25 cm vs. 1 cm dataset), and initial condition improved the estimation of the observed data.
- Transport properties such as dispersivity will be estimated.
- Estimation of parameters will be used to test different uncertainty analysis methods (e.g., null-space Monte Carlo method and p-field simulation).

**Reference:** Yoon, H., Zhang, C., Werth, C.J., Valocchi, A.J., and Webb, A.G. 2008. Numerical simulation of water flow in three dimensional heterogeneous porous media observed in a magnetic resonance imaging experiment. Water Resources Research. 44. W06405.

## ACKNOWLEDGMENT

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