Groundwater Model Parameter Estimation with Simultaneous and Sequential Use of Hydraulic Head and Travel Time Measurements

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Mohsen Kheirabadi

B.S., K. N. Toosi University of Technology, 2005

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At the University of Connecticut
2018
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Mohsen Kheirabadi

2018
Groundwater Model Parameter Estimation with Simultaneous and Sequential Use of Hydraulic Head and Travel Time Measurements

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University of Connecticut
2018
ACKNOWLEDGEMENTS

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I would especially like to thank Mrs. Vivian E. Sovinsky for her kind support during my thesis. She shared her expertise with me very generously and I have learned a lot from her.

I would also like to thank my fellow lab-mates for their stimulating discussions, supporting my work with careful comments and encouraging me and giving me their priceless advice on how to deal with obstacles both in research and my student life.

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Abstract

This study is an effort to investigate two parameter estimation approaches in groundwater modeling, sequential and combined use of flow and transport observations. Most researchers postulate that simultaneous use of flow and transport observations would be more beneficial in parameter estimation; however, some others raise questions about this approach. They argue that due to the differing geological properties of aquifers and consequently different mathematical basis of groundwater flow and transport equations, simultaneous use of these two types of observations might not be useful in all cases. Despite the fact that parameter estimation or inverse modeling is not a new method in groundwater modeling, most modelers tend to use forward modeling to estimate parameters. In this research a synthetic heterogeneous K-field is created using SGeMS Sequential Gaussian Simulation. The model synthetic observations obtained from forward models MODFLOW and MODPATH are used in the process of parameter estimation using PEST++. In order to explore the model and improve it, various scenarios have been defined and tested. Applying the principle of parsimony, complexity is added gradually in each scenario. The sequential approach performs two calibrations: a flow calibration using head observations followed by transport calibration using travel time observations. Both sets of observations are applied simultaneously in a single calibration run in the combined approach. Comparing the estimated parameters of hydraulic conductivity and porosity with their corresponding synthetic ground truth reality values shows that in most cases better results were achieved for both hydraulic conductivity and porosity while applying the combined approach. However, the combined approach was more complex to use, very time-consuming and presented an additional challenge in finding the best weight for each run.
1 Introduction

1.1 Background

1.1.1 Importance of Groundwater Sustainability

Groundwater is the water found underground in soil pore spaces and in the fractures of rock formations. This body of water is dynamically evolving, with water that constantly flows into the system by recharge from precipitation and leaves the system through natural or man-made mechanisms. Understanding groundwater discharge and recharge mechanisms is essential for allowing us to work out how much groundwater we can pump and where we can pump it from in order to minimize our impact on the ecosystem.

In the US, groundwater provides half of the drinking water (U.S. Geographical Survey, Groundwater Use in the United States) and it also plays a vital role in agriculture and industry, therefore using appropriate groundwater management and well-studied protection techniques would enable sustainable use of this highly valuable water resource. Groundwater is used for drinking, washing, food production, industrial activities and to sustain ecosystems. Billions of people around the world rely on groundwater for their water supply. Meanwhile, there is a great number of plants and animals that also depend on groundwater for their survival.

Each groundwater system is unique, because the system is dependent upon external hydro-meteorological factors as well as structural formation of its container which is called aquifer. However, the total amount of water inflowing, outflowing, and being stored in the system must be conserved. This specific definition which is derived from the law of conservation of mass is called water budget. We perform water budget calculations in order to account for quantitative changes in a groundwater system. However, groundwater sustainability is not only dependent on the
quantity of water in the system but is affected by human activities like excessive withdrawals, irrigation, domestic and industrial usages that could have detrimental effects on the quality of groundwater.

Human activities can change the components of the water budget. Pre-development of a groundwater budget using natural conditions of the system before human activities can be useful in some cases but it has a lot of limitations (Bredehoeft et al., 1982). For example, at the beginning of exploiting an aquifer, if the rate of groundwater withdrawal does not exceed the rate of natural recharge, we might say the system is sustainable and exploiting the system is safe but in this case we neglected any changes both in aquifer properties and environment during the time due to the groundwater withdrawal and other activities. Therefore, pre-development of groundwater budget is not realistic and it should be consider dynamically.

This concept of neglecting dynamic changes has been referred to as the "Water-Budget Myth" (Bredehoeft et al., 1982). It is a myth because first, human activities change the system and second, it is an oversimplification of the information which will negatively affect any decision making.

1.1.2 Types of Groundwater Modeling

Groundwater modeling provides a powerful tool for groundwater management, protection and remediation. Models in general are simplification of reality in order to facilitate the investigation and prediction of the behavior of a system. The challenge is that simplification of reality would have an adverse effect on the ability of a model to provide sufficiently accurate model outputs.
Regardless of simplicity or complexity of a model, models may produce wrong results if they are not properly designed; therefore, choosing the right model based upon our needs and our available information is of great importance. Groundwater models can be classified into three categories: physical, analogue and mathematical. Solution of mathematical models can be either analytical or numerical (Baalousha, 2008). Analytical models need less data but they are limited to simple applications while numerical models can handle much more sophisticated situations. Thanks to the technological advances in the past decades, numerical models became more popular and there are so many different software programs available to groundwater modelers. Two commonly used numerical approaches in groundwater modeling are “finite differences” and “finite elements”. Each of them has its advantages and disadvantages. Choosing an appropriate modeling approach along with other factors like boundary conditions, initial conditions, time and space discretization, and quality of data would affect the results. Regardless of the type of model being used, the stepwise methodology of forward groundwater modeling is as follows. Figure 1 illustrates these steps in a clear fashion. Defining the objective of the model is the first step. Then data collection and conceptual modeling are the next steps. Mathematical modeling and model design are at the core of any numerical modeling but perhaps model calibration is the most time consuming part of the model. After model completion, verification and sensitivity analysis must be conducted to make sure that the model will still be valid under different conditions.
Figure 1 - General stepwise flowchart of groundwater modeling (Courtesy of Baalousha, 2008)
1.2 Objectives

This study is the continuation of a previous study by Vivian Sovinsky (2017) which posed the following question “does the optimized reality more closely resemble the true reality when multiple observations are applied?” To answer this question previous work focused on comparing two key approaches to automated calibration: (1) the sequential approach: use of a single type of observation for driving the estimates of each input parameter one at a time and (2) the combined approach: using multiple types of observations together to drive the calibration process. In the work presented here the objectives can be listed as:

- Investigating the hypothesis under a different and more complete set of scenarios
- Investigating the effect of groundwater abstraction (pumping well) on the existing flow regime and observing its effect on the optimization results
- Investigating the effect of observation well density and distribution pattern
- Observing the model capability on handling prediction model outputs while different types of errors are present.

1.3 Implementation of sequential and combined approaches in inverse modeling

There is significant body of research supporting simultaneous use of transport and flow-system observations (Wagner and Gorelick, 1987; Gailey et al., 1991; Sonnenborg et al., 1996; Anderman and Hill, 1999). These researchers argue that when we use transport information such as concentration observations, we could more easily obtain flow and transport parameters because (1) concentrations or travel times are sensitive to velocities and (2) direction and magnitude of
velocities depend on the properties of the model. Wagner and Gorelick (1987) were the first to develop a coupled estimation model and they used a synthetic example to test their methodology.

Numerous studies have been published on the subject of coupled estimation of flow and transport parameters in order to show simultaneous estimation of parameters produce more accurate outputs. The major reason behind that is while we apply coupled estimation strategy, we reduce uncertainty of the model compared to a sequential approach whereby subsets of the observations (e.g., only heads or only travel times, or only concentrations) are used to estimate both flow and transport parameters (e.g., Gailey et al., 1991; Sonnenborg et al., 1996; Barlebo et al., 1998; Anderman and Hill, 1999). However, other researchers (e.g., Jacques et al., 2002) emphasize that in some cases a sequential estimation strategy might produce the same results as those from a coupled inverse procedure.

An early study by Strecker and Chu questioned the sequential approach, stating that this approach amplifies the error in transport model outputs because solving the model for K based on head data, and then using those K parameters in the subsequent transport model increases the uncertainty of the model (Strecker and Chu, 1986).

In an attempt to estimate model parameters in a groundwater quality management project Wagner and Gorelick (1987) applied simultaneous consideration of modeled and observed concentrations and hydraulic heads in a homogeneous K synthetic reality. His approach is then successfully applied to a Gloucester Landfill study in Ottawa, Canada (Gailey et al., 1991). Wagner and Gorelick (1987) and Gailey et al. (1991) - applied statistical analysis to estimate parameter values. Sonnenborg et al. (1996) has conducted a field study similar to Gloucester in a waste residue site and used a combined approach to find flow and transport parameters.
Voss states that the differences in the analytical basis of groundwater flow and groundwater transport make the combination of these sets of observations questionable. Voss believes a flow calibration using only hydraulic heads will query more information of the aquifer than the transport calibration while models addressing transport calibration tend to obtain most of the information in high K channels. Two factors contribute to this: (1) flow distributes in both low K and high K areas thus the observations of flow has information of all area, and (2) the flow equation resembles the diffusion equation (Voss, 2011a).

1.4 Scope of Work

In this work a geostatistics software program (SGeMS) along with python programming language is used to create a synthetic heterogeneous hydraulic conductivity field. Then using a relationship of porosity to K, porosity values for this field are created. In order to create the observations for the calibration tests, forward model runs of the flow and transport models are performed (Table 1). After that, inverse models are set up to estimate parameters of the model in two different approaches. The following tables illustrate the modeling steps in a more sensible way.

<table>
<thead>
<tr>
<th>MODFLOW</th>
<th>MODPATH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Create Head Observations Using K-field</td>
<td>Creating Travel Times Using Existing Information (Modeled Heads) and Porosity Reality</td>
</tr>
</tbody>
</table>
Table 2- Inverse Model Runs to Estimate Aquifer Needed Parameters Using PEST++, MODFLOW and MODPATH

<table>
<thead>
<tr>
<th>Model Set (Estimated Parameters)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sequential Runs</strong></td>
</tr>
<tr>
<td>✓ Sequential Flow (3Ks)</td>
</tr>
<tr>
<td>✓ Sequential Transport (4 Porosities)</td>
</tr>
<tr>
<td><strong>Combined Runs</strong></td>
</tr>
<tr>
<td>✓ Combined Flow and Transport (3 Ks and 4 Porosities)</td>
</tr>
</tbody>
</table>
2 Methodology

2.1 Groundwater Modeling and Governing Equations

2.1.1 Hydraulic Properties of Aquifers

In order to understand how water flows through an underground layer of permeable rock, sediment (usually sand or gravel), or soil, we need to know a few specific geologic properties of these subsurface systems (USGS, 2016). This research focuses on two key properties; hydraulic conductivity and porosity. Hydraulic conductivity can be defined as a parameter that describes the ease with which water can move through porous media or fractures under certain hydraulic head variation. Porosity is a ratio of the volume of voids over the total volume. In reality the geological composition of a very small area of interest may vary greatly, causing significant diversity of properties across the 3D space. So it seems impractical to find geological properties of an area very accurately, in contrast, in typical field studies, scientists and engineers try to find hydraulic heads and tracer concentrations of an area of interest and then using statistical and mathematical techniques to make a good, descriptive model.

Due to the recent decades technological advances in sophisticate techniques like X-ray computed tomography (CT) system, we are able to obtain very accurate internal visualization of geo-materials in three dimensions (Cnudde et al., 2011). Although, it is a non-destructive way, to find a meaningful structural information of an area, many small samples are needed to be scanned and combined to make a representative sample. This technique is still in progress, very expensive and time consuming and except for specific cases, it is not economically justifiable.

The data shortage in hydro-geological studies led scientists to develop some techniques to compensate for the lack of input properties values in their models. As we will see in the following sections, in typical groundwater models the geological properties are inputs while outputs reflect
field measurements. Therefore, comparing model outputs and field data leads us to the field of inverse modeling study.

2.1.2 Input parameters

2.1.2.1 Hydraulic Conductivity

Hydraulic conductivity is basically a measurement of how well an aquifer can transmit water. Different materials transfer water differently at faster or slower rates. It depends on permeability and permeability itself depends on pore size and pore connectivity.

Hydraulic conductivity, symbolically represented as K provides an indication of how much water (volume per time) will pass through a unit area of the aquifer, for each unit difference in hydraulic head. K in essence depends on the structural properties of a porous media which vary greatly. The hydraulic conductivities span several orders of magnitude (Bear, 1972).

2.1.2.2 Porosity

Porosity is a quantity that shows how much space is available for water to move through the porous media. While these open spaces (trapped in grains or fractures in rocks) are connected with other pores, water is allowed to flow through the media. In hydrology this interconnected porosity is called “effective porosity” which is essential to find velocities, travel times and contaminant transport analysis (Strecker and Chu, 1986)

2.1.3 Output/Measurements

2.1.3.1 Hydraulic Heads

In groundwater modeling, hydraulic head measurements represent the summation of pressure head and elevation head exerted by the water (Bear, 1972). In confined aquifers, this is also called piezometric head or surface which expresses virtual water level or in other words, where
the water would rise to if given an outlet. Thus, a piezometer can be used to measure these pressure heads, which are expressed in units of length.

2.1.3.2 Travel Times

Travel time (also referred to as residence time) is a measure of how much time a particle takes to travel a specific length of a medium or how much time a particle spends in it. The term residence time emphasizes that the particle resides in the specified aquifer (or a specified space) for a specified length of time. There are at least three different residence times used in civil and environmental engineering literature, namely, the turn-over time or flushing time, the mean age, and the transit time or travel time. In this work we apply the travel time method that indicates travel from one boundary (the first column) of the aquifer to our observation points.

2.1.4 Flow Modeling

In 1856, Henry Darcy, a French engineer, discovered a mathematical relationship that governs the flow of groundwater through granular media or in general the flow of other fluids through permeable material. Based on Darcy’s law for 1D groundwater flow:

\[ Q = -KA \frac{dh}{dl} \]  

\[ \frac{dh}{dK} = -\frac{Q}{K^2A} \frac{l}{l} \]

\( Q \) is the groundwater flowrate \([\text{L}^3\text{T}^{-1}]\)

\( K \) is the hydraulic conductivity \([\text{LT}^{-1}]\)
\( A \) is the cross sectional aquifer area perpendicular to flow \([L^2]\)

\( \frac{dh}{dl} \) is the hydraulic gradient [dimensionless]

\( l \) distance along an axis, therefore parallel to the direction of flow \([L]\)

Hydraulic head is a nonlinear function of \( K \) because \( \frac{dh}{dK} \) is a function of \( K \) (Equation 2). As this equation implies sensitivity of hydraulic heads with respect to aquifer properties, such as \( K \) is a function of the aquifer properties and flows.

Darcy’s law is stating that volumetric flowrate through groundwater system is proportional to cross-section area, the hydraulic gradient and hydraulic conductivity being the coefficient of this proportionality. Hydraulic conductivity is a function of the properties of the medium (soil) and the fluid (water). This implies that it is specific for each soil and it allows us to estimate how much water is going to flow through a soil based on cross-section area and hydraulic gradient.

On the other hand we know that conservation of mass simply states that the difference between inflows and outflows must be equal to the change in storage.

\[ \text{Flows in} - \text{Flows out} = \text{Change in Storage} \]

By application of Darcy’s law and mass conservation, and assuming XYZ axes are aligned with the principal axes of anisotropy:

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = S_x \frac{\partial h}{\partial t}
\]

Including a source/sink term \( R^* \) (positive for recharge and negative for pumping), which is defined as the volume of inflow per unit volume of aquifer per unit of time \([T^{-1}]\):

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = S_x \frac{\partial h}{\partial t} + R^*
\]
\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) + R^* = S_t \frac{\partial h}{\partial t}
\]

This is an equation describing 3D transient flow through a saturated anisotropic porous medium. This is a basis of all groundwater modeling for a confined aquifer. A confined aquifer is always saturated and it is assumed to be anisotropic and that is why we have different K in different directions.

In this research a modular finite-difference flow model (USGS MODFLOW-2005) which is a computer code that solves the groundwater flow equation is used to simulate the flow of groundwater through the aquifer. MODFLOW is a modular program which utilizes the capabilities of object-oriented programming. Different options, called packages, can be turned on and off while using MODFLOW. In this 3D Groundwater Model the subsurface volume of interest is divided into cells where each cell is assumed to have constant property values, such as hydraulic conductivity and porosity. MODFLOW provides finite difference models for groundwater flow and includes numerous optional modules, such as modeling interactions with surface water, transport modeling, and groundwater management (Harbaugh, 2005).
Hydraulic conductivity for each cell must be specified for the equations to be solved. Sometimes only a few hydraulic conductivity field values are available. Therefore, we need to use one of the estimation methods to find the unknown K field values. Three common approaches are (1) estimating an average K for the entire volume, (2) estimating zones of homogeneous K values using expert knowledge of the field site, and (3) creating statistical simulations to provide a statistical distribution (or combination of distributions) of K.

Eggleston et al. compared multiple stochastic simulations: Sequential Gaussian, simulated annealing, and kriging (Eggleston et al., 1996). Some of the statistical approaches, like the Sequential Gaussian Simulation used in this work use known spatial relationships of K, and can produce a heterogeneous K field that reflects known spatial continuity (Isaacs and Srivastava, 1989). Another statistical approach, transition probability indicator simulation (TPROGS) has been shown to more closely simulate the geology of high-K facies (Lee et al., 2007).
2.1.5 Transport Modeling

Transport modeling is a post-processing of the flow model results. A particle-tracking post-processing program (i.e. MODPATH) which has been designed to work with MODFLOW outputs (Pollock, 2012) is applied to find travel-times. Flow simulation outputs, heads and flows are inputs in MODPATH software program. Using flows and effective porosities, we can find pore velocities which are essential to determine both pathways and travel times. For this work, we applied a backward simulation of the motion of particles from the observation locations back to the first column of the model. This backward time is equal to the time for the particle to travel forward with the flow of groundwater (if we exclude dispersion in forward modeling and just consider advective transport) from the starting boundary of the model to the center of each observation well. Dispersion was not included in the transport model in order to isolate the effects of porosity; multiple transport processes would have complicated the influence of porosity values (Sovinsky, 2017).

2.2 Modeling Software and Hardware

This section shows the main software programs and computing resources which have been utilized for this research. Basic descriptions along with version are listed here. More details could be found online.
**Table 3- Software programs used in this study**

<table>
<thead>
<tr>
<th>Application</th>
<th>Description</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>SGeMS</td>
<td>Stanford Geostatistical Modeling Software</td>
<td>V2.5b</td>
</tr>
<tr>
<td>MODFLOW</td>
<td>USGS’s 3-D Finite Difference Groundwater Model</td>
<td>1.0.9</td>
</tr>
<tr>
<td>MODPATH</td>
<td>USGS’s particle-tracking post-processing program that uses MODFLOW output files to perform transport calculations.</td>
<td>Modpath6.0</td>
</tr>
<tr>
<td>Pest++</td>
<td>Watermark Numerical Computing’s Parameter Estimation (Calibration Program) – author John Doherty</td>
<td>3.5+fixes</td>
</tr>
</tbody>
</table>

**Table 4- Programming language and libraries (packages) utilized in this study**

<table>
<thead>
<tr>
<th>Programming Language &amp; Libraries</th>
<th>Description</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Python</td>
<td>Anaconda Package with Jupyter notebook IDE</td>
<td>Version 3.5.1</td>
</tr>
<tr>
<td>Flopy</td>
<td>Python library to create, run, and post-process MODFLOW-based models using a programming interface.</td>
<td>Version 3.2.5</td>
</tr>
<tr>
<td>Numpy</td>
<td>Python Library for array operations and manipulation</td>
<td>Version 1.11</td>
</tr>
<tr>
<td>Pandas</td>
<td>Python Library for data analysis</td>
<td>Version 0.19.0</td>
</tr>
</tbody>
</table>
### Table 5- Hardware/OS utilized for this study

<table>
<thead>
<tr>
<th>Hardware/OS</th>
<th>Description</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asus K45VD</td>
<td>Anaconda Package with Jupyter notebook IDE</td>
<td>IceCool Technology</td>
</tr>
<tr>
<td>Intel® Core™ i5 3210M-Processor</td>
<td>a fast dual-core processor for laptops based on the Ivy Bridge architecture</td>
<td>3M Cache, 3.10 GHz</td>
</tr>
<tr>
<td>Windows - 7 Professional OS</td>
<td>64-bit</td>
<td>Service Pack 1</td>
</tr>
</tbody>
</table>

PEST and PEST++ Version 3 (Doherty, 2014, 2015) both provide a feature called “Yet Another Run Manager” (YAMR), which can be invoked through a windows command. A short windows command file is required to specify directory names and files that need to be copied into each of the four directories. The final results of the calibration run are found in the master file. The main PEST++ process runs in the master directory which delegates runs of the models (e.g., MODFLOW) in each of the slave directories, so there can be three simultaneous executions of MODFLOW—each of which passes their results back to the main PEST++ process running in the master directory (Sovinsky, 2017).

2.3 Creating Synthetic Reality

2.3.1 Create Synthetic K-field

The Stanford Geostatistical Modeling Software (SGeMs) was used to create a synthetic reality for a 2D hydraulic conductivity (K) field. Among different options that SGeMs provides, Sequential Gaussian Simulation has been chosen. It creates a log normal distribution of hydraulic conductivity while maximizing entropy and conforming to a pre-selected variogram. Variogram is an equation that relates variance as a function of distance between pairs of lnK values or lag distance. Table 6
illust"rates geostatistical and simulation parameters that we used to create a Gaussian variogram
and a synthetic K-field.

\textit{Table 6- Variogram and simulation parameters}

<table>
<thead>
<tr>
<th>Parameters and Symbols</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range ( a )</td>
<td>distance where variogram is 95% of sill value</td>
<td>200m</td>
</tr>
<tr>
<td>Variance (sill s) or ( \sigma^2 )</td>
<td>variance at lags &gt; range</td>
<td>0.4 (lnK-K in m/d)</td>
</tr>
<tr>
<td>Mean ( \mu )</td>
<td>mean of simulated lnK’s</td>
<td>1.8 (lnK-K in m/d)</td>
</tr>
<tr>
<td>Nugget ( n ) or ( C_0 )</td>
<td>variance at lag of 0</td>
<td>0</td>
</tr>
<tr>
<td>Variogram Curve</td>
<td>Choices: Exponential, Gaussian, Spherical</td>
<td>Gaussian</td>
</tr>
</tbody>
</table>

The kriging mean and variance are required to generate a Gaussian field using Sequential Gaussian
Simulation procedure. It allows us to honor the Gaussian variogram equation given by

\[
\gamma(h) = C_0 + \sigma^2 (1 - \exp(-\frac{3h^2}{a^2}))
\]  \hspace{1cm} (5)

Where \( h \) is the lag distance, \( a \) is the practical range, \( \sigma^2 \) is the variance (or sill), \( \mu \) is the mean of simulated LnKs and \( C_0 \) is the nugget.
The output of SGeMS sequential Gaussian simulation is a synthetic reality. It resembles the hydraulic conductivity of our aquifer in each cell. The generated field dimensions are 500m by 1000 and each cell is 1m by 1m.
Using SGeMS sequential Gaussian simulation and setting the sill of the variogram to the value of 1 (Bohling, 2007) a set of 10 standard normal distributions of LnK has been generated and one was chosen as the lnK distribution for the synthetic reality. This approach allows us to be more flexible in post-processing of simulation outputs.

We chose post-simulation adjustment strategy. It means first, we defined mean = 0 and variance = 1 and then a python script executed within SGeMS allowed us to back-transform the outputs to a chosen mean and variance. The mean used was lnK=1.8 and the variance was lnK = 0.4. This script also converted lnK values back to K. The final Ks file is the file that we need to export to our Jupyter notebook in next steps.

2.3.2 Create Synthetic Porosity-field

In this study we use the Las Cruces experimental plot of porosity and hydraulic conductivity developed by Wierenga et al. (1989). The Las Cruces site refers to a trench located approximately 40 km northeast of Las Cruces, New Mexico. This trench was dug to provide samples for
characterization of hydrologic properties (e.g., bulk density, porosity, particle-size distribution, saturated hydraulic conductivity and water retention parameters).

A realistic range of effective porosity (0.2 to 0.4) was mapped to the range of LnK using the following equation:

\[ Y = 0.0983 \cdot X + 0.1426 \]  

(6)

Where Y is porosity and X is LnK.

Equation (6) is slightly different than the linear regression line in order to provide enough variation in estimated porosity values. In this way we slightly eased estimation of porosity values for our model.

*Figure 5- Porosity and Hydraulic conductivity from Las Cruces, NM (Wierenga et al. 1989)*
In this study four zones of hydraulic conductivities were created and then zones of porosity were mapped following these four zones of Ks. The average hydraulic conductivity and porosity were computed and used in next steps as a metric to compare our estimation with real values. These average values are shown in Table 7.

Table 7- Average values for hydraulic conductivity and porosity

<table>
<thead>
<tr>
<th>Hydraulic Conductivity</th>
<th>Min &lt; K1 &lt; 4.0</th>
<th>2.904</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.0 &lt; K2 &lt; 7.0</td>
<td>5.512</td>
</tr>
<tr>
<td></td>
<td>7.0 &lt; K3 &lt; 10.0</td>
<td>8.298</td>
</tr>
<tr>
<td></td>
<td>10.0 &lt; K4 &lt; Max</td>
<td>12.088</td>
</tr>
<tr>
<td>Porosity</td>
<td>Por 1</td>
<td>0.244</td>
</tr>
<tr>
<td></td>
<td>Por 2</td>
<td>0.309</td>
</tr>
<tr>
<td></td>
<td>Por 3</td>
<td>0.350</td>
</tr>
<tr>
<td></td>
<td>Por 4</td>
<td>0.386</td>
</tr>
</tbody>
</table>

Figure 6-Porosity Zones (columns and rows in meter)
2.3.3 Establish Boundary Conditions

To satisfy the governing equations which are the basis of MODFLOW (Harbaugh, 2005) we need to define boundary conditions. In addition to values of $K$ for each cell, MODFLOW requires any boundary conditions such as no-flow boundaries, specified heads or flows, and any fluxes into or out of cells. For this model a confined aquifer with a depth of 30 meters was specified. To the left and right constant head boundaries were defined, in order to create flow from left to right. The upper and lower boundaries are defined as no-flow boundaries and the top and bottom of the single layer model is automatically no-flow due to being defined as confined (Sovinsky, 2017).

![Aquifer Boundary Conditions](Image)

*Figure 7- Establish boundary conditions for aquifer simulation (Courtesy of Sovinsky, 2017)*
2.3.4 Assumptions and Limitations

There are some inherent assumptions along with a few imposed limitations in this research approach.

1) Firm boundary conditions are specified. Without knowing exact fluxes of water at boundaries in field situations, which is the real case, often complicates the estimation of input parameters, therefore modelers need to simulate the boundaries as either no-flow or an estimated specified head or flow.

2) The granularity of the cells are assumed to be constant across cells, thus it is sufficient to capture the aquifer behavior without introducing an amount of model structural error.

3) The reality is synthetic – so results could be specific to this reality.

4) In field situations sampling density is often far less than our model and also uneven distributed which in our simulation this limitation has been violated in first three scenarios.

5) The number of parameters that needs to be estimated is much less than the number of observations. So this calibration may behave better due to this issue.

6) Some research (Lee et al., 2007; Eggleston et al., 1996) considers the Sequential Gaussian Simulation for a K field to be an unlikely representation of a truly existing heterogeneous K-reality because this simulation does not produce sufficient connection among high-K values which are typically found in heterogeneous aquifers.

2.4 Creating Different Scenarios

In previous study (Sovinsky, 2017), there are 200 equally spaced observations. This sampling density is not typical in field situation, because first there exist areas that are difficult to sample, second often samples are unevenly distributed. Addressing this limitation and also adding
more complexity to the system, four different scenarios were defined. In each scenario, complexity is added step by step and all the runs are repeated. In first scenario, we have 200 observation wells evenly distributed across the field, second is identical to the first one but a pumping well is added at the location 200m and 700m with the pumping rate equal to 500 m$^3$/day. Third scenario is similar to the second but with less observation wells, i.e. 50 instead of 200, and in the last scenario we added all the complexities and created a field with 50 observation wells, randomly distributed plus a pumping well. Figure 8 illustrates these 4 scenarios.

Figure 8- Configuration of observation wells in different scenarios
2.5 Creating Observations (Forward Modeling)

2.5.1 Creating Flow Model Observations: Heads

The following shows the key process steps to create hydraulic heads in forward modeling. Moreover, Figure 9 helps us to understand the process in a clearer way. To accomplish this process MODFLOW was applied inside a Python script.

1) Import synthetic K-field generated using SGeMS

2) Set up boundary conditions and convergence criteria for MODFLOW model. In this study we use Flopy package which is a library for connecting python programming language with USGS computational groundwater flow models such as MODFLOW and MODPATH.

   NOTE: except scenario A, in other scenario we need to set up a pumping well in the field.

3) Run MODFLOW inside the Python script. Output is a set of 500 by 1000 hydraulic heads.

4) Select equally or randomly spaced observations, depending on different scenarios

5) Add random errors to the observations. This step is an optional step. In next chapter we discuss about inherent errors of using “zone of constant value” method that automatically are introduced into our process.

   NOTE: for optional adding errors, we chose stddev = 0.1m for heads.

6) Open a flat file such as text file, write the observation values in that file and save it. In this form they can be easily imported into PEST++ control file.
2.5.2 Creating Transport Model Observations: Travel Times

The following shows the key process steps to create travel times in forward modeling. Moreover, Figure 10 illustrates the process in a more clear way. To accomplish this process MODFLOW and MODPATH were applied inside a single Python script.

![Diagram](image)

*Figure 9- Creating head observations using synthetic K-field, Python script and MODFLOW software*

1) Import synthetic K-field generated using SGeMS

2) Set up boundary conditions and convergence criteria for MODFLOW model. In this study we use Flopy package which is a library for connecting python programming language with USGS computational groundwater flow models such as MODFLOW and MODPATH.

   NOTE: except scenario A, in other scenario we need to set up pumping well in the field.

3) Run MODFLOW inside the Python script. Output is a set of 500 by 1000 hydraulic heads.
4) Set up transport simulation boundary conditions and introducing MODFLOW outputs to the MODPATH, which are cell budgets, hydraulic heads and discretization file. In this study we used “endpoint” simulation method. Tracking backward travel of particles from observation points to the starting locations, MODPATH is able to find travel times for each particle.

5) Run MODPATH. Output are travel times for a set of particles backtracked from observation points to the starting points.

6) Using Pandas, extract travel times.

7) Add random errors to the travel time observations. This step is optional.

   NOTE: for optional adding errors, we chose stddev = 10 days for travel times.

8) Open a flat file such as text file, write the observation values in that file and save it. In this form they can be easily imported into PEST++ control file.
Figure 10- Creating travel time observations using synthetic porosity values, MODFLOW outputs, Python programming language and MODPATH, computational groundwater model for particle tracking
2.6 Model Calibration

2.6.1 Calibration Goals and Techniques

The process of finding parameter values that produce results that closely match the observations is called calibration. In automatic calibration, the objective is parameter estimation or inverse modeling which allows the model to quantitatively connect observations (measured values), parameters (hydraulic conductivities and porosities), and predictions (modeled values) through an optimization process. If the values of the resultant estimates more closely reflect the true aquifer geology that is relevant to the water dynamics, models can become better predictors of future outputs (Hill and Tiedeman, 2007; Doherty, 2015). It is common to use the term “inverse modeling” and “parameter estimation” interchangeably in groundwater modeling literatures.

Some researchers believe that inverse modeling has greater capability in uncertainty evaluation, sensitivity analysis and data prediction, especially when dealing with very complex models (Poeter and Hill, 1997; Faunt et al., 2004). Quantifying the quality of calibration is important to modelers and resource managers. Calibration methods include both manual and automated approaches. Unlike governmental agencies and some firms, often environmental consulting companies prefer to use manual approaches due to their simplicity. However, the manual method can be time-consuming and may introduce significant error due to the subjectivity of the approach (Hill and Tiedeman, 2007). Popularity of trial-and-error method might be due to the lack of user-friendliness of the inverse methods and the perception that these methods require more time than trial-and-error calibration method. Using trial and error approach to calibrate a model, we compare observed and simulated values, e.g. hydraulic heads, concentrations or flows, which is time consuming and subjective, thus in this approach, comparing a calibrated model to another one in terms of goodness of calibration is very difficult.
Despite great advances in geophysical data collection and analysis (e.g., Eppstein and Dougherty, 1996; Hyndman and Gorelick, 1996; Lebbe, 1999; Dam and Christensen, 2003) data scarcity is still a big problem in groundwater modeling. There are some methods that suggest to ignore the nonlinearity and/or carefully ignore some of the complexity of the models (Kitanidis (1997) and Sun (1994)) in order to obtain models that provide well enough estimated values. Overcoming this issue, regression has been introduced into groundwater modeling literature in the 1970s (reviewed by McLaughlin and Townley, 1996) which is a powerful tool for calibration when we are going to address complexity of the physical systems and scarcity of data.

In some models, parameter estimation is a linear problem, i.e. the observed values are linear function of the parameters, but in most cases the inverse model problem is nonlinear and more effort is needed to solve them. Parameterization in groundwater inverse modeling mostly is focused on hydraulic conductivity or transmissivity. There are many approaches in terms of addressing this issue. The most complex parameterizations are cell- or pixel-based methods in which parameters are defined for each pixel or element and regularization is used to provide stable solution (e.g., see Tikhonov and Arsenin, 1977; Clifton and Neuman, 1982; Backus, 1988; McLaughlin and Townley, 1996). The simplest parameterization method is to assume homogeneity of the model domain and introduce one parameter to specify hydraulic conductivity or porosity throughout the model. Between the two extreme parameterization methods, there are some others in which they benefit of interpolation methods such as pilot points (RamaRoa et al., 1995; Doherty, 2003; Moore and Doherty, 2005, 2006) or zonation designed based upon constant value for each zone.

Estimating hydraulic conductivity in a groundwater modeling is a nonlinear problem and PEST++ uses nonlinear regression method to solve this problem. PEST++ is an automated
approach to calibration developed by John Doherty at Watermark Numerical Computing (Doherty 2014; Doherty, 2015). PEST++ is related to the original program PEST; PEST++ was designed to be easier to apply than PEST and to address issues with highly parameterized inverse modeling.

2.6.2 Objective Function, Observed and Simulated Values

In the context of automatic calibration, the objective function is a measure that represents how well observed and simulated values match in a model. The lower the value of the objective function the better the fit of observed and simulated values. Methods such as regression that help us find the minimum objective function are called calibration methods and the resulting parameter values are optimized values. In this study, weighted least-squares regression using PEST++ is applied. The weighted least-squares objective function with a diagonal weight matrix, $\phi$, can be expressed as:

$$\phi = \sum_{i=1}^{NH} \omega_h [y_h - y'_h]^2 + \sum_{j=1}^{NT} \omega_j [y_{t_j} - y'_{t_j}]^2$$

(7)

Where $NH = \text{the number of hydraulic-head observations}$;

$NT = \text{the number of travel-time observations}$;

$y_h = \text{the } i\text{-th observed hydraulic-head being matched by the regression}$;

$y'_h = \text{the } i\text{-th simulated hydraulic-head that corresponds to } i\text{-th observed hydraulic-head}$

$y_{t_j} = \text{the } j\text{-th observed travel-time being matched by the regression}$;

$y'_{t_j} = \text{the } j\text{-th simulated travel-time that corresponds to } j\text{-th observed travel-time}$;
\( \omega_{hi} \) = the weight for the \( i \)-th head observation;

\( \omega_{ji} \) = the weight for the \( j \)-th travel-time

For a full weight matrix, the least-squares objective function can be written as

\[
\phi = [y - y']^T \omega [y - y'] = e^T \omega e
\]

(8)

Where \( \omega \) is the weight matrix, \( y \) is a vector of observations, \( y' \) is a vector of simulated values and \( e \) is a vector of residuals.

In sequential approach first we use hydraulic heads to find corresponding parameter values for hydraulic conductivities, and then we use this information along with travel times to find porosities. However, in combined approach we apply both hydraulic heads and travel times simultaneously to find parameter values. When we use combined approach we need to implement weights for at least two obvious reasons. First, different types of observations and simulated values (hydraulic heads vs. travel times), are not in a same scale, therefore we need to use weights to remove the misleading effects of different magnitudes. Second, some observations are less reliable in a sense that we are less confident about their accuracy than others, as a result we need to reduce their effects in the objective function. In other words, we use weights to provide unbiased observations for our model, because if an observation (or prior information) is biased, the model is likely to be biased.

Mathematically, weights can be expressed as:

For a diagonal weight matrix \( \omega \propto 1/\sigma_i^2 \)  
(9)

For a full weight matrix \( \omega^{1/2} \propto V(e)^{-1} \)  
(10)
Where \( \propto \) means “proportional to,” \( \varepsilon \) is a vector of true errors, \( \sigma_i^2 \) is the variance of the true error of observation \( i \), and \( V(\varepsilon) \) is the variance-covariance matrix of the true errors, with variance along the diagonal and covariances off the diagonal.

As can be seen, the weight of each point is inversely proportional to the variance of that point’s dataset. We do not have a dataset for each point in this study, therefore we need to guess weights for observations and run the model and proceed based upon trial-and-error to find the best weights while we use the combined approach. This is a problematic part of this approach, because sometimes it requires a lot of trials to find the best weights.

In this research, the tool PEST++ was used. This software program applies following steps to perform non-linear regression:

1) Computes Jacobian Matrix: this step is prior to each iteration. Elements of this matrix provide sensitivity of each model output to changes in each parameter (Doherty 2015).

\[
J = \begin{bmatrix}
\frac{\partial z_1}{\partial k_1} & \frac{\partial z_1}{\partial k_2} & \cdots & \frac{\partial z_1}{\partial k_m} \\
\frac{\partial z_2}{\partial k_1} & \frac{\partial z_2}{\partial k_2} & \cdots & \frac{\partial z_2}{\partial k_m} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial z_n}{\partial k_1} & \frac{\partial z_n}{\partial k_2} & \cdots & \frac{\partial z_n}{\partial k_m}
\end{bmatrix}
\]  

(11)

Where:

Each model output \( o_i = z_i \ [k] \); \( i \) from 1 to \( n \) for \( n \) outputs

And each parameter \( k_j \); \( j \) from 1 to \( m \) for \( m \) parameters (Doherty, 2015).
2) At each PEST++ iteration, multiple vectors are computed based on varying the (non-negative) damping factor \( \lambda \); each vector represents a different set of parameter values. PEST++ invokes the appropriate groundwater model(s) to run for each set of parameters and then chooses the result which has the lowest Phi. The runs of the groundwater model required for a single iteration is equal to the number of parameters plus 1, thus if estimating 7 parameters, 8 runs are required.

3) At each iteration: computed set of values (determined by identifying the best vector) and the corresponding Phi are compared with the results of earlier iterations to see if convergence has occurred. Two main convergence criteria that used in this study are

a) Phi Convergence – the objective function no longer changes beyond a specified interval.
b) Parameter Convergence – the parameters no longer change beyond a specified interval.

When the chosen convergence criteria are met, the calibration is completed.

2.6.3 Sequential Flow and Transport Calibration

In sequential approach, first calibration of flow model is performed to estimate \( K \) values using only hydraulic head observations. The outputs of the first calibration are needed for the next calibration step. In second calibration step, transport model is run using only travel time observations and it estimates porosity values.

Objective functions for these two calibration steps are as follows. In first equation head observations are compared to simulated heads, and in the second travel time observations are compared to modeled travel times.

\[
\Phi_h = \sum (H_{\text{orig}} - H_{\text{model}})^2
\]

\[
\Phi_t = \sum (T_{\text{orig}} - T_{\text{model}})^2
\]

The following figures illustrate these two steps of sequential approach. The alternative to sequential approach is combined approach which merges two calibration steps and uses both hydraulic heads and travel times at the same time.
Figure 12 - Sequential approach flowchart, step 1 - find K values

Figure 13 - Sequential approach flowchart, step 2 - find porosity values
2.6.4 Combined Flow and Transport Calibration

In combined approach flow and transport models are applied simultaneously to obtain optimum Ks and porosities. Both hydraulic head and travel time observations which are forward model outputs, are used for comparison to simulated heads and travel times. Minimizing the weighted sum of the squared residuals provides optimum Ks and porosities.

Figure 14- Combined approach flow chart – as shown in figure PEST++ is integrated with both MODFLOW and MODPATH. The value of Ks estimated by MODFLOW and PEST++ in each iteration are used by MODPATH and PEST++ sequentially. This loop continues up to completion of calibration process.
The objective function for this calibration approach is as follows. In this approach hydraulic head and travel time observations are compared to modeled outputs simultaneously. Minimum $\Phi$ provides the optimum values for $K_s$ and porosities.

$$\phi = \sum \omega_h \left[ H_{\text{orig}} - H_{\text{model}} \right]^2 + \sum \omega_t \left[ T_{\text{orig}} - T_{\text{model}} \right]^2$$

(14)

Where $H$ is hydraulic head, $T$ is travel time, $\omega_h$ and $\omega_t$ are weight for heads and travel times respectively.
3 Results and Discussion

3.1 Comparison of results while there is no added random error

Hydraulic conductivity and porosity values are the outputs of sequential and combined calibration approaches. The objective in any groundwater modeling calibration is to modify these parameters such that the hydraulic heads and travel times we get from flow and transport models match reality. In other words, the objective of calibration is to look at the heads and travel times we get from modeling and compare them with the heads and travel times we measured and try to make them as close as possible. The measured values represent reality and model is our attempt to generate reality. While measured and modeled values are closed enough, we can say we have a good model.

The most common methods in optimization are gradient methods because they apply the gradient of the objective function surface to proceed and find the minimum. PEST++ software program uses Levenberg–Marquardt Algorithm (LMA) to find optimum solutions. This method is also known as the damped least-squares method and it is basically a modified version of Gauss-Newton method. This method is capable of solving non-linear least squares problems. However, such as many fitting algorithms, the LMA finds only a local minimum, but it is more robust than many others in a sense that even if it starts very far from optimum values in many cases it is able to find a solution.

In this study two different approaches have been investigated. In sequential approach first, using flow model and PEST++, optimum K values are estimated, then using those optimized values transport model along with PEST++ are applied to estimate porosities. In contrast, combined approach utilizes flow and transport model simultaneously. In each iteration the results
of hydraulic conductivity calibration are the inputs for porosity calibration and this process continues until all the convergence criteria are met.

One problem we encountered in this study was non-uniqueness of the models. In order to alleviate the effects of this issue, the hydraulic conductivity of zone 3 was fixed. The reason for choosing zone 3 is that the pumping well is located at this zone, thus it could be easily estimated using pumping test information for example. Porosity for zone 3 was allowed to vary and be estimated.

Avoiding adding any prior information, initial values were chosen far away from optimum (average observed) values. For hydraulic conductivity optimum values in meters per day are 2.904, 5.512, 8.298 and 12.089 and initial values also in meters per day are 1.5, 3.0, fixed = 8.298 and 8 respectively. For porosities optimum values are 0.244, 0.309, 0.350 and 0.386 and initial values are 0.20, 0.25, 0.30 and 0.35, respectively.

Other than investigating two different approaches, in order to have a model that can predict accurately enough in different situations, we developed our model and investigated it in different scenarios.

The following figures relate the results of two different approaches while we do not add extra random errors to observation values. As section 2-4 shows Case-A has 200 observation wells, evenly distributed across the field. Case-B is identical to Case-A but it has a discharge well at the location 200m and 700m with the pumping rate of 500 m³/day. Case-C has 50 observation wells and a pumping well identical to the discharge well in Case-B and Case-D has 50 observation wells randomly distributed across the field and the same pumping well as Case-B and C.
Figure 15 - Case A, comparing the results of two different approaches for hydraulic conductivity estimation (without adding random errors)

Figure 16 - Case A, comparing the results of two different approaches for porosity estimation (without adding random errors)
Figure 17- Case B, comparing the results of two different approaches for hydraulic conductivity estimation (without adding random errors)

Figure 18- Case B, comparing the results of two different approaches for porosity estimation (without adding random errors)
Figure 19 - Case C, comparing the results of two different approaches for hydraulic conductivity estimation (without adding random errors)

Figure 20 - Case C, comparing the results of two different approaches for porosity estimation (without adding random errors)
Figure 21 - Case D, comparing the results of two different approaches for hydraulic conductivity estimation (without adding random errors)

![Case D (w/o) Hydraulic Conductivity](image)

<table>
<thead>
<tr>
<th></th>
<th>HK 1</th>
<th>HK 2</th>
<th>HK 3</th>
<th>HK 4</th>
<th>NRMSE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target</td>
<td>2.904</td>
<td>5.512</td>
<td>8.298</td>
<td>12.089</td>
<td></td>
</tr>
<tr>
<td>Sequential</td>
<td>2.494</td>
<td>5.825</td>
<td>8.298</td>
<td>13.22</td>
<td>8.33</td>
</tr>
<tr>
<td>Combined</td>
<td>2.486</td>
<td>5.81</td>
<td>8.298</td>
<td>13.16</td>
<td>7.98</td>
</tr>
</tbody>
</table>

Figure 22 - Case D, comparing the results of two different approaches for porosity estimation (without adding random errors)

![Case D (w/o) Porosity](image)

<table>
<thead>
<tr>
<th></th>
<th>Por 1</th>
<th>Por 2</th>
<th>Por 3</th>
<th>Por 4</th>
<th>NRMSE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target</td>
<td>0.244</td>
<td>0.309</td>
<td>0.350</td>
<td>0.386</td>
<td></td>
</tr>
<tr>
<td>Sequential</td>
<td>0.245</td>
<td>0.324</td>
<td>0.332</td>
<td>0.405</td>
<td>1.50</td>
</tr>
<tr>
<td>Combined</td>
<td>0.232</td>
<td>0.332</td>
<td>0.341</td>
<td>0.396</td>
<td>1.40</td>
</tr>
</tbody>
</table>
Comparing the final results obtained from the sequential and combined approaches it is demonstrated that better estimated values are obtained when the combined approach is applied.

It should be noted here that while grouping K values into “constant value zones” inherent errors are introduced in to the model. These errors are the result of taking the average of the values of Ks and porosities in each zone. The following table shows the amount of errors introduced by this approach for each zone. It is clear that the errors are higher for hydraulic conductivity than porosity in this model.

Table 8- Inherent errors while "zone of constant value" method is used

<table>
<thead>
<tr>
<th>Zone</th>
<th>Mean (HK.s)</th>
<th>Std (HK.s)</th>
<th>% (Std/Mean)</th>
<th>Mean (Por.s)</th>
<th>Std (Por.s)</th>
<th>% (Std/Mean)</th>
<th># Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone 1</td>
<td>2.904</td>
<td>0.678</td>
<td>23.3%</td>
<td>0.244</td>
<td>0.025</td>
<td>10.4%</td>
<td>113871</td>
</tr>
<tr>
<td>Zone 2</td>
<td>5.612</td>
<td>0.841</td>
<td>15.3%</td>
<td>0.309</td>
<td>0.015</td>
<td>4.9%</td>
<td>213638</td>
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<tr>
<td>Zone 3</td>
<td>8.298</td>
<td>0.827</td>
<td>10.0%</td>
<td>0.360</td>
<td>0.010</td>
<td>2.8%</td>
<td>116977</td>
</tr>
<tr>
<td>Zone 4</td>
<td>12.089</td>
<td>1.902</td>
<td>15.7%</td>
<td>0.387</td>
<td>0.014</td>
<td>3.7%</td>
<td>54515</td>
</tr>
</tbody>
</table>

3.2 Comparison of results while there are added random errors

The following figures illustrate the results of calibration in two different approaches while random errors are added to observations. These values are stddev= 0.1m for heads and stddev=10 days for travel times. Comparing the results of two approaches show that (1) in general, the combined approach is able to estimate parameters more accurately which is consistent with our expectations; (2) The relative improvement of the combined approach is better for porosity estimation; (3) In both cases (with or without adding random errors) comparing scenarios B and C shows that the effect of reducing sampling density has deteriorating effect on hydraulic conductivity estimations but for porosities we cannot conclude if reducing the sampling density
has a negative or positive effect on the accuracy of estimation; (4) In combined approach each run takes time approximately 3.5 times more than sequential approach; moreover, to find the best weights in combined approach we need to have 5 to 10 different test runs. Mathematically there is no guarantee of finding the best weights when we use trial-and-error methods; (5) In general, we can argue that the improvements using combined approach compared to sequential approach for both cases (with and without adding random errors) are not significant considering the efforts that need to be expended to accomplish the tasks.
Figure 23 - Case A, comparing the results of two different approaches for hydraulic conductivity estimation (with adding random errors).

Figure 24 - Case A, comparing the results of two different approaches for porosity estimation (with adding random errors).
Figure 25- Case B, comparing the results of two different approaches for hydraulic conductivity estimation (with adding random errors)

Figure 26- Case B, comparing the results of two different approaches for porosity estimation (with adding random errors)
Figure 27- Case C, comparing the results of two different approaches for hydraulic conductivity estimation (with adding random errors)

Figure 28- Case C, comparing the results of two different approaches for porosity estimation (with adding random errors)
Figure 29- Case D, comparing the results of two different approaches for hydraulic conductivity estimation (with adding random errors)

<table>
<thead>
<tr>
<th></th>
<th>HK 1</th>
<th>HK 2</th>
<th>HK 3</th>
<th>HK 4</th>
<th>NRMSE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target</td>
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<td>5.512</td>
<td>8.298</td>
<td>12.089</td>
<td></td>
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<tr>
<td>Sequential</td>
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<td>6.061</td>
<td>8.298</td>
<td>15.417</td>
<td>21.11</td>
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<tr>
<td>Combined</td>
<td>2.492</td>
<td>5.821</td>
<td>8.298</td>
<td>13.491</td>
<td>9.92</td>
</tr>
</tbody>
</table>

Figure 30- Case D, comparing the results of two different approaches for porosity estimation (with adding random errors)

<table>
<thead>
<tr>
<th></th>
<th>Por 1</th>
<th>Por 2</th>
<th>Por 3</th>
<th>Por 4</th>
<th>NRMSE (%)</th>
</tr>
</thead>
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<td>Target</td>
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<tr>
<td>Sequential</td>
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<td>0.345</td>
<td>0.411</td>
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<tr>
<td>Combined</td>
<td>0.233</td>
<td>0.331</td>
<td>0.341</td>
<td>0.403</td>
<td>4.82</td>
</tr>
</tbody>
</table>
3.3 Sensitivity, Evaluating Model Fit and time-cost

Sensitivities can be defined as the derivatives of simulated values with respect to the model parameters. That is,

\[
\left( \frac{\partial y'_i}{\partial b_j} \right)_{b}
\]

Where \( y'_i \) is defined as simulated value that corresponds to an observation and \( b_j \) is the \( j \)-th parameter. Subscribes \( i \) and \( j \) are important because in non-linear problems the sensitivities for different parameter values are different, that is the reason these sensitivities are called local sensitivities (Saltelli et al., 2000). PEST++ approximates sensitivities in three different schemes, forward, backward or central differences. For example the forward-difference approximation is:

\[
\left( \frac{\partial y'_i}{\partial b_j} \right)_{b} \approx \left( \frac{y'_i(b + \Delta b) - y'_i(b)}{\Delta b} \right)
\]

Sensitivities are very useful to indicate the importance of the observations in the estimation of parameter values. However, there is a problem when comparing the relative importance of different observations. The problem is that sensitivities are in the units of the simulated value divided by the units of the parameter. For example, in a groundwater model, the simulated values might be hydraulic heads measured in meters, or travel times measured in days and parameters might be hydraulic conductivity measured in meters per day, or porosity in which is dimensionless. This incompatibility makes the comparison between different sensitivities extremely difficult. In order to address this issue different methods of scaling are used. PEST++ accomplishes this task automatically.
The value of objective functions is rarely used for comparisons between different models and scenarios. In contrast, in this study, a single value (NRMSE, normalized root mean squared error) has been specified to provide an overall model fit evaluation. Using this value, we can quickly assess how well a model matches all the observations and prior information.

Another way to analyze model fit is to utilize graphs of simulated vs observed values. The following figures show simulated vs observed head observations for Case-A with adding random errors. As it can be seen, this display of the data does not reveal which approach provides a better model fit. That is why NRMSE is needed, a single value that helps to quickly find the goodness of fit in each case.

![Figure 31: Sequential approach - Plot of modeled vs measured hydraulic heads in Case-A with adding random errors](image-url)
Another method of showing results is to plot residuals vs. modeled values. This method applied on hydraulic heads of Case-A with adding errors. In this method, we are able to create a trend line and compare this trend line with the one created for another approach and interpret the results in a mathematical fashion using a single value. Comparing $R^2$ for two approaches indicates that the residuals of the sequential flow model are less biased with respect to modeled heads.

Figure 32- Combined approach - Plot of modeled vs measured hydraulic heads in Case-A with adding random errors
Figure 33 - Sequential flow results showing residuals vs modeled heads

Figure 34 - Combined flow results showing residuals vs modeled heads
Figure 36 shows contour plots of hydraulic heads for two scenarios (Cases A and D). As it can be seen, comparing the accuracy of two approaches based upon the results plotted in the form of contours is challenging. Even for circumstances like case D with the addition of random errors which the accuracy of the estimation of hydraulic conductivities are significantly different for two approaches (NRMSE 21.11% for sequential vs NRMSE 9.92% for combined) differentiating the results and determining which approach is better using contour plots is challenging.

Figure 35- Comparing sequential and combined outputs with observed values – Case A – with adding random errors
Theoretically, time complexity of both sequential and combined approaches is similar in Python scripts but the average time required for the combined approach to complete a run is approximately 3.5 times more than sequential approach, (approximately 7hr compared to 2hr). This issue is due to the complexity of the combined simulation model which requires MODFLOW and MODPATH run sequentially in each iteration.
4 Conclusions

4.1 Summary

The idea of this study is aimed to achieve more effective use of data. In our groundwater model, the model inputs (hydraulic conductivity and porosity) that need to be estimated are distributed spatially, therefore there are numerous parameter values in our model domain. In reality, however, a limited number of samples is available for modelers. Dealing with this limitation would be really challenging so that we need to choose a limited number of parameters which they are good representatives of the model domain.

In this study two inverse approaches have been investigated in an attempt to estimate parameter values more efficiently using parameter estimator software, PEST++ along with Python programming language. These two approaches are sequential and combined. There are numerous field and simulation studies supporting simultaneous estimation of model parameters but some other researchers raised questions about the combined approach, stating the differences in the analytical basis of groundwater flow and groundwater transport make the combining of these sets of observations problematic. (Voss, 2011).

In order to have a closer look at this issue, a synthetic heterogeneous K-field was created using SGeMS Sequential Gaussian Simulation. Then we created a confined aquifer by applying “zone of constant value” method, defining boundary conditions and implementing other assumptions. In forward modeling, MODFLOW and MODPATH were used to generate synthetic observations. Meanwhile, different scenarios have been defined and complexities have been added step by step. The process of calibration was implemented using PEST++ parameter estimation software for both sequential and combined approaches. PEST++ is able to go through the process
of solving non-linear regression equations and use sensitivity matrix and find best estimates automatically.

Although, the results of two set of calibration runs indicate combined approach consistently provides better estimated values, these differences are not significant. The higher run time and complexity of combined approach along with challenges in finding the best set of weights indicate that using the sequential approach in the complex groundwater modeling problems could be also considered.

4.2 Future Work

This research has a great potential and could be tested and expanded around these following topics: 1) different boundary conditions, 2) variogram and geostatistical simulation type, 3) sampling density, 4) comparing the effect of different randomly distributed samples, 5) grid resolution and 3D simulation, 6) adding random errors on observation values.

Another exiting field of research, related to this study is to investigate pilot-point approach. Although this method of calibration is increasingly common, few academic works have been done on its mathematical implications and/or implementation of this highly parameterized inverse method in hydro-geologic modeling.

We hope this study will encourage other researchers to explore these methods and make them more robust.
5 References

A Vanishing Aquifer: What happens when the water runs out? National Geographic Society.


Cambridge, UK: Cambridge University Press.


Research, 32 (4), 925–938.


U.S. Geographical Survey. The USGS Water Science School, Groundwater Use in the United


