SIMULATION AND OPTIMIZATION MODELS TO EVALUATE PERFORMANCE OF AQUIFER

STORAGE AND RECOVERY WELLS IN FRESH WATER AQUIFERS

by

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Simulation and Optimization Models to Evaluate Performance of Aquifer Storage and Recovery Wells in Fresh Water Aquifers

by

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The study employed simulation, statistical, and optimization models to evaluate the performance of an aquifer storage and recovery (ASR) system in a fresh water aquifer in Utah. Recovery effectiveness (REN) is the performance index of the studied ASR system, which equals the injectate proportion that the same wells can recover. The study presented a methodology employing groundwater flow and contaminant transport modeling to estimate REN. In order to distinguish the injected water from native groundwater, the transport model assumed an imaginary non-reactive contamination in the injected water, and quantified the recoverable “contamination” during extraction periods. The study also assessed the effect of different screen interval schemes for improving REN, and introduced vertical heterogeneity as a crucial factor on REN.
The study developed a transferable software to 1) rapidly estimate REN for different hydrogeological and operational factors, and 2) perform a sensitivity analysis of the factors affecting REN. The software circumvents the need to prepare and run computationally intensive transport simulations. The study also showed that the system's overall REN is more than 95%, if the wells extract three times their injection volume in the same year of injection (typically within 3-4 months after injection). Extracting merely the same volume as injectate would achieve REN not more than 75% for most wells. This highlighted the importance of having pre-existing water rights to achieve a high REN. Finally, the study employed optimization models to aid managing the ASR system for the conditions of storing the injected water in the aquifer for a year. The optimization models find the optimal ASR wells and their optimal decision variables (injection rate and extraction duration) to maximize the system's overall REN with the least extraction volume and cost. The results categorized the system’s wells into three rankings based on their recovery effectiveness.
Simulation and Optimization Models to Evaluate Performance of Aquifer Storage and Recovery Wells in Fresh Water Aquifers

Ali Forghani

Aquifer storage and recovery (ASR) involves artificially recharging an aquifer through well(s) using surplus water for later recovery in high-demand months. The operators of the studied ASR system developed the system as a means of receiving additional water rights to supplement their pre-existing water rights for extraction in dry months. However, the region's water regulators define the performance of this ASR system as the amount of the injected water that is recoverable from the same wells during extraction periods. The study proposes recovery effectiveness (REN) as the performance index of this ASR system. REN equals the injectate proportion that the same wells can recover. Quantifying the system's achievable REN is required to determine the amount of the additional water rights. Similarity between the injected water and native groundwater, however, prevents an accurate REN estimation using on-field techniques. This necessitates the use of computer modeling for estimating REN in this system. The study employs simulation, statistical, and optimization models to quantify and maximize REN in the studied ASR system in Utah.
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CHAPTER 1
INTRODUCTION

Imbalance between water supply and demand is a challenging problem for water managers in many parts of the world (Shamsai and Forghani, 2011; Banihabib et al. 2017). This makes satisfying peak water demands a critical objective, especially in dry months in arid regions. Aquifer storage and recovery (ASR) is a technique to balance water supply and demand for sustainable water resources management. This technique involves treating the excess surface water and recharging it into aquifers for later recovery when demand exceeds water supply. Thus, ASR is an alternative to the construction of larger storage and treatment facilities that are otherwise required (Pyne, 1995).

Water managers can implement ASR systems in both fresh water aquifers (FWAs) and saline or brackish aquifers. ASR systems in FWAs differ from ASR in saline aquifers not only because of the different physical phenomena involved, but also because of the different criteria to quantify their performances. Modeling studies by Ward et al. (2009) present dimensionless parameters to describe ASR systems performance in saline aquifers.

This dissertation addresses an ASR system in a FWA operated by the Jordan Valley Water Conservancy District (JVWCD) in Salt Lake County, Utah (Figure 1-1). Satisfying increasing peak demands in hot summer months has been a challenge for the JVWCD for years. Before implementing the ASR project, the JVWCD was satisfying much of its peak demand by importing water through two aqueducts. The JVWCD had to meet the
rest of the peak demands by groundwater pumping from the already declining groundwater aquifer. The JVWCD implemented many studies to investigate options for increasing delivery during peak demand times. They first studied the feasibility of constructing a surface reservoir within Salt Lake County, but the study concluded that reservoir seepage losses would be substantial (Dames & Moore, 1983). Another alternative was constructing an additional aqueduct conveyance, but this option was analyzed to be very expensive (SLCWCD 1996).

Figure 1-1. The JVWCD ASR project Area
The JVWCD started a demonstration ASR project during 1992-1994 using one injection well, one extraction well in the downstream vicinity of the injection well, and one injection/extraction well. The demonstration project accomplished many findings regarding the best manners of operating an ASR system and treating surface water for underground injection, especially to minimize clogging. Injection testing also confirmed a high specific capacity of the aquifer for storing the anticipated recharge volume. The concept of ASR was deemed feasible in the region and eventually the JVWCD started the full scale ASR project with 14 injection/extraction wells on the east side of Salt Lake Valley in 2000 (Figure 1-1).

The sources of surface water for storage in the aquifer are flows in local streams that were unutilized in the past. Prior to injection, the surface water undergoes full treatment to comply with all drinking water regulations. Two JVWCD treatment plants use conventional flocculation, sedimentation, filtration, and disinfection processes. The JVWCD uses these treated waters to meet existing municipal and industrial demands. The JVWCD injects the remainder of the treated water underground for later recovery. Therefore, the volume of extra surface water for aquifer storage varies annually based on the volumes of stream flow and municipal and industrial demands. Because the JVWCD has no competitors for the extra surface water, it can potentially store any portion of that water based on the ASR system’s capacity (written communication with Alan Packard at the JVWCD).
The JVWCD uses the existing drinking water distribution system to convey water to the injection wells and injects the water using the system’s pressure. The quality of the recharged water is very high and similar in chemical constituents to the native groundwater. The stored water is recovered for municipal and industrial purposes (SLCWCD 1996).

The groundwater system underlying the Salt lake Valley consists of quaternary-age basin fill. The valley is surrounded by mountains on the east, south, west, and northeast and by Great Salt Lake on the northwest. The basin fill consists of unconsolidated to semi-consolidated sediments with interbeds of clay, silt, sand, and gravel and lenses of sand and gravel. The basin fill source is sediment from adjacent mountains. Generally, the sediments are coarser near the mountains and finer in the central and northern parts of the valley. Discontinuous fine-grained layers in the central part of the basin create a semi-confined aquifer. This semi-confined aquifer consists of deposits of clay, silt, sand, and gravel. A shallow unconfined aquifer overlies the fine-grained layers in the center of the valley. Fine-grained layers are absent on the margins of the valley which is the primary recharge area for the valley. The surrounding mountains consist of consolidated rock with substantial secondary porosity but with negligible primary porosity (Lambert 1995). Section 2-2 provides more details of the extent and hydrogeology of the aquifer for artificial recharge.

The JVWCD ASR wells are all screened either in the confined zone in the center of the valley or in unconfined zones near the valley margins. The ASR wells have a 40 or
50cm casing diameter. Table 1-1 shows background gradient, vertically-averaged horizontal hydraulic conductivity \((K_h)\), vertically-averaged Darcian velocity (the product of gradient and \(K_h\)), maximum injection rate, and extraction rate of 14 JVWCD ASR wells. The aquifer porosity is estimated to be 0.3 near all wells.

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<thead>
<tr>
<th>Name</th>
<th>Gradient</th>
<th>(K_h) (m/d)</th>
<th>Darcian velocity (m/d)</th>
<th>Max Injection Rate (m(^3)/d)</th>
<th>Extraction rate (m(^3)/d)</th>
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<tr>
<td>SLCWCD3</td>
<td>0.0049</td>
<td>23</td>
<td>0.113</td>
<td>6260</td>
<td>8710</td>
</tr>
<tr>
<td>SLCWCD4</td>
<td>0.0014</td>
<td>18</td>
<td>0.025</td>
<td>8170</td>
<td>23980</td>
</tr>
<tr>
<td>SLCWCD5</td>
<td>0.0015</td>
<td>20</td>
<td>0.030</td>
<td>5460</td>
<td>7830</td>
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<tr>
<td>SLCWCD6</td>
<td>0.0012</td>
<td>7</td>
<td>0.008</td>
<td>3820</td>
<td>7100</td>
</tr>
<tr>
<td>SLCWCD8</td>
<td>0.0007</td>
<td>5</td>
<td>0.004</td>
<td>4920</td>
<td>11010</td>
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<tr>
<td>SLCWCD9</td>
<td>0.0008</td>
<td>7</td>
<td>0.006</td>
<td>2720</td>
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<tr>
<td>SLCWCD15</td>
<td>0.0022</td>
<td>30</td>
<td>0.066</td>
<td>5460</td>
<td>9810</td>
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<td>SLCWCD18</td>
<td>0.0019</td>
<td>20</td>
<td>0.038</td>
<td>5460</td>
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<td>0.0038</td>
<td>40</td>
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<tr>
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<td>0.0013</td>
<td>21</td>
<td>0.027</td>
<td>8170</td>
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<tr>
<td>SLCWCD33</td>
<td>0.004</td>
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<td>0.016</td>
<td>7630</td>
<td>21800</td>
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<td>0.0018</td>
<td>24</td>
<td>0.043</td>
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<td>24250</td>
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<tr>
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<td>0.012</td>
<td>5460</td>
<td>14660</td>
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</table>

The JVWCD developed this ASR system as a means of receiving additional water rights for extraction in dry months by injecting excess surface water in wet months. However, the Utah Division of Water Rights (UDWR), which regulates water rights for the region, determines the additional water rights based upon the recoverable injectate proportion. In other words, the performance of the studied ASR system is measured as
the injectate proportion that the same wells can recover during subsequent extraction
periods.

Similarity in quality between injected water and native groundwater prevents an
accurate estimation of the system's performance using on-field techniques. The JVWCD
tried extensive testing to track recoverable injectate by monitoring concentrations of
natural tracers. However, the results were uncertain and provided only general trends
(SLCWCD 1996). This necessitates the use of modeling to estimate the system's
performance, especially to fulfill the accuracy needed for water right negotiations
between JVWCD and UDWR. So far, no studies have evaluated the performance of such
an ASR system in a freshwater aquifer.

Chapter 2 defines recovery effectiveness (REN) as the performance index of the
studied ASR system:

\[
\text{REN} = \frac{V_{E_{\text{Inj}}}}{V_i}
\]  

(1)

where \(V_{E_{\text{Inj}}}\) is the volume of the injectate contained within the extracted water, and \(V_i\) is
the volume of the injected water.

This chapter presents a methodology employing groundwater flow and transport
modeling to quantify REN for one of the JVWCD wells named SLC8. In the absence of
density contrasts between injected water and native groundwater, it is not required to
use density-dependent groundwater models. In the JVWCD ASR system, for specified
ASR operational settings (i.e. injection/extraction rates and durations), background
seepage velocity is the predominant factor that can affect REN. Therefore, the methodology uses MODFLOW (McDonald and Harbaugh, 1988) and MT3DMS (Zheng and Wang 1999) models for groundwater flow and transport simulations.

Because of the similarity between injected water and native groundwater, in the MT3DMS model, the injected water is assumed as an imaginary non-reactive “contamination” to distinguish it from the native groundwater. The injected water is modeled with an arbitrary concentration of 100ppm while assuming zero concentration for native groundwater. MT3DMS tracks the injected "contamination" during an ASR operation and computes the amount of the injected "contamination" that the same ASR well can recover. The ratio of extracted "contamination" to the total injected "contamination" gives an estimation of REN (Equation 1).

Chapter 2 also presents a procedure to prepare a sufficiently refined local model capable of considering site-specific hydrogeology and aquifer heterogeneity—the factors that can significantly affect the seepage velocity and the ASR system’s performance. To prepare the refined local models, the study employs a two-stage grid refinement technique on a USGS-calibrated MODFLOW regional model (Lambert 1995). The procedure provides vertically and horizontally refined models needed for an accurate estimation of REN while being computationally inexpensive. The results of this chapter reveal that preparing sufficiently refined models is essential in REN estimation. Using models that are more horizontally-refined increases REN almost linearly within the tested range.
This chapter also assesses the effect of different screen interval schemes for improving REN. Furthermore, this chapter investigates the degree of importance of vertical heterogeneity on REN in FWA. To do so, the results of SLC8, which has a relatively low background gradient, are compared with another JVWCD ASR well (SLC22) located in an area with a steeper gradient (Figure 1-2).

![Map of ASR wells SLC8 and SLC22](image)

Figure 1-2. The locations of ASR wells SLC8 and SLC22 used in chapter 2

As mentioned, Chapter 2 presents a methodology to estimate REN using MODFLOW-MT3DMS models. Utilizing these models, however, can be challenging. Developing MODFLOW-MT3DMS models can be cumbersome, and simulation times can
be very long. This prevents analyzing multiple ASR scenarios in a manageable time frame. To overcome this difficulty, Chapter 3 presents the development of a software that rapidly estimates REN without the need to prepare and run MODFLOW-MT3DMS models. This also enables performing sensitivity analysis of different factors affecting REN.

As substitute simulators, the software invokes two trained artificial neural networks (ANNs). The ANNs estimate REN for two injectate storage conditions: 1) allowing minimal storage of injected water (i.e. extraction begins immediately after injection), and 2) allowing one year storage of injected water (i.e. extraction begins after storing the injectate in an aquifer for 12 months). Both ANNs assume injecting into an aquifer for two months, which is a reasonable injection duration for many ASR systems including the JVWCD system.

The dataset needed to train and validate the ANNs is obtained from 10,000 MODFLOW-MT3DMS simulations for the two injectate storage conditions. A dataset with 10,000 simulations is sufficient because it provided a negligible improvement for the accuracy of the ANN models in comparison to a dataset with only 5,000 simulations. Dataset inputs include all factors that can significantly affect REN in freshwater aquifers. These seven factors are background hydraulic gradient, hydraulic conductivity, screen interval length, porosity, longitudinal dispersivity, injection rate, and extraction rate. Dataset outputs are computed RENs for each 15 days of extraction up to 120 days. To handle the large number of MODFLOW-MT3DMS simulations, the study uses parallel
processing by the message passing interface (MPI) technique (Gropp et al. 2014) to run a large number of simulations in parallel.

The developed ANNs in Chapter 3 are generalized—they are useful to estimate REN not only for the JVWCD ASR system, but for any other ASR system whose parameters are within the range of the values used to develop the ANNs. In addition, Chapter 3 presents the development of a graphical user interface (GUI) to facilitate using the ANN models, and also to perform sensitivity analysis of different factors on REN.

Chapter 4 presents a procedure using transport and statistical models to evaluate the overall REN for the JVWCD ASR system based on the current operational scheme. The procedure addresses two objectives: 1) estimating overall REN using MODFLOW-MT3DMS models by simulating the operation of all ASR wells (Figure 1-3) simultaneously, and 2) statistically identifying significant parameters affecting REN, and identifying the most recovery-effective wells.

To address the first objective, this chapter uses a 5-year monthly refined model with the January 2009 heads as the starting heads. The calibrated aquifer parameters from the USGS MODFLOW model (Lambert 1995) are used as the basis to develop the flow model. In order to ensure the validity of these aquifer parameters to simulate the groundwater system in Salt Lake Valley under current hydrological stresses, this chapter also performs a model verification analysis. To do so, the USGS model, which has been calibrated for the years 1969 to 1992, is extended with the updated stresses
representing hydrologic conditions from 1993 to 2014. Then, the accuracy of the 1993-2014 model is evaluated by comparing its results with observed heads in the region.

![Street-view map of all ASR wells](image)

Figure 1-3. Street-view map of all ASR wells

To address the second objective, transport modeling results are employed in the multivariate adaptive regression splines (MARS) regression technique (Friedman 1991). MARS is a non-parametric regression technique that provides results in a form similar to multiple linear regressions (MLR) while revealing nonlinearities. Unlike MLR, which
provides one slope for each significant variable, MARS provides piecewise linear relations between significant variables and REN. MARS also identifies the range for each significant variable that provides maximum RENs.

Chapter 5 presents a simulation-optimization model to aid managing the JVWCD system for yearly storage of injected water. The yearly storage condition assumes injecting within year 1 and extracting within year 2 (after 12 months of water storage in the aquifer). Three considered objectives within the optimization model are 1) maximizing the system’s overall REN, 2) minimizing the system’s extraction volume within year 2, and 3) minimizing pumping costs. Two decision variables of each well are injection rate and extraction duration.

The optimization model with Objectives 1 and 2 provides optimal solutions (the optimal wells to operate and their optimal decision variables) representing the trade-offs between the system’s extracted volume versus the system’s achievable REN. The optimization model with objectives 1 to 3 updates the results after considering the effect of pumping costs. This chapter’s results categorize the 14 JVWCD ASR wells into three rankings based on their recovery effectiveness for yearly injectate storage. These rankings are used to propose operational guidelines for the JVWCD system in order to maximize the system’s overall REN.

The proposed model in Chapter 5 couples the multi-objective genetic algorithm NSGA2 with the neural networks developed in Chapter 3. Using the ANNs allows performing many REN simulations in the optimization model. By comparing the ANN-
computed RENs with the RENs obtained from a regional multi-layer MODFLOW-MT3DMS model, Chapter 5 also presents the applicability of the neural networks to estimate REN in many ASR systems worldwide, even for partially penetrating wells screened in multiple strata.

In summary, this dissertation employs simulation, statistical, and optimization models to evaluate REN in ASR systems in freshwater aquifers. Chapter 2 investigates the importance of screen interval designs on achievable REN in individual wells. Chapter 3 presents the development of a surrogate simulator to rapidly estimate REN. Whereas Chapter 4 estimates the overall REN in the JVWCD ASR system for the current operational settings (which involves a significant amount of extraction in the same year of injection), Chapter 5 estimates achievable REN for the system if extracting after one year of injectate storage in the aquifer.
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CHAPTER 2

PERFORMANCE ASSESSMENT OF ASR WELLS IN FRESHWATER AQUIFERS USING A TWO-STAGE REFINEMENT TECHNIQUE

Abstract

We present a methodology to quantify the performance of an aquifer storage and recovery (ASR) system developed for water right purposes in a freshwater aquifer (FWA). The operator of the studied ASR system desires to receive permission to add the injected water volume to preexisting water rights. However, for water right allocations, the water regulators define the performance of this ASR system as the amount of the injected water that is recoverable from the same ASR well during extraction periods. We propose the new recovery effectiveness (REN) system performance index and employ transport modeling to quantify REN. Modeling must achieve the accuracy needed for this water right negotiation, and must consider the predominant effect of background seepage velocity on REN in the studied ASR system. Therefore, we apply a two-stage grid refinement procedure on a calibrated regional model to prepare an accurate high-resolution local model. The local model uses transient monthly specified perimeter boundary conditions and background stress, considers aquifer heterogeneities, and is computationally efficient. Simulations present the crucial importance of model horizontal discretization on computed REN. Results also show that screening in less permeable layers, if it does not hamper the functionality of the ASR well during injection and extraction, can improve REN. The importance of avoiding screening in higher
permeability layers increases as the background gradient increases. Therefore, the study reveals that vertical heterogeneity can have a crucial impact on REN for the wells located in the regions with high background gradient.

2-1-Introduction

Imbalance between water supply and demand is a challenging problem for water managers in many parts of the world. Satisfying peak water demands is critically important, especially during dry months in arid regions. Water managers design water treatment and storage facilities for a specific water demand. Enlarging the facilities to satisfy increased peak demand can significantly increase the project’s costs. Aquifer storage and recovery (ASR) is an alternative to constructing larger surface water storage and treatment facilities. ASR involves recharging excess surface water (perhaps after some treatment in a water treatment facility) into an aquifer for later recovery. ASR helps to balance water supply and demand for sustainable water resources management (Pyne 1995).

Water managers can implement ASR systems in both fresh water aquifers (FWAs) (Forghani and Peralta 2017a) and saline or brackish aquifers (Ward et al. 2009; Brown et al. 2016). ASR systems in FWAs differ from ASR in saline aquifers not only because of different physical phenomena involved, but also because of regulatory and water right issues that can affect the criteria to quantify their performances. For ASR
systems in saline aquifers, the criterion to measure system’s performance is recovery efficiency \( (\text{RE}_{\text{Saline}}) \). Equation 1 quantifies RE.

\[
\text{RE}_{\text{Saline}} = \frac{V_E}{V_I} \tag{1}
\]

\( V_E \) is the volume of extracted water with suitable quality for intended use (i.e. usually with Total Dissolved Solids, TDS, lower than allowed TDS), and \( V_I \) is the volume of injected water. During an ASR extraction period, the TDS of the recovered water increases until it reaches the allowed TDS. Operators then halt extraction (because water with excess TDS is unusable) and use Equation 1 to compute RE. Density difference between injected water and ambient (or native) groundwater causes buoyancy of the injected water. This buoyancy can result in the early capture of saline ambient groundwater and can reduce RE (Pyne 1995 and Ward et al. 2009). Therefore, most ASR modeling studies in saline aquifers employ a variable-density groundwater flow model coupled with a transport model. The ability to measure \( V_E \) and \( V_I \) and to compute \( \text{RE}_{\text{Saline}} \) in the field, enables ASR managers to calibrate aquifer parameters for simulation models and to evaluate RE for other scenarios (Pavelic et al. 2006).

Performance evaluation of ASR systems in FWAs requires a different procedure than ASR systems in saline aquifers. Equation 1 uses the quality of the extracted water as a limiting factor for extraction. However, this equation is not useful for ASR systems in FWAs where injected water and ambient groundwater have similar acceptable quality and there is little potential for adverse geochemical activity.
Water managers define performance of ASR systems in FWAs based on project needs or regulatory issues. For example, Ebrahim et al. (2015) evaluate the feasibility of an ASR system in a coastal aquifer in Oman where the major concern is seawater intrusion. After an injection to the aquifer, the extraction from the freshwater aquifer continues as long as the gradient is not from the sea inland. Whether the extracted water actually was injected water or native water is unimportant for quantifying the performance of this system.

The ASR system in a FWA we address here differs—managers must know how much of the injected water is recoverable from the same well. The Jordan Valley Water Conservancy District (JVWCD) began operating a full-scale ASR project in a FWA in Utah, USA in the year 2000 (Figure 2-1a). The JVWCD developed this ASR system as a means of receiving additional water rights for groundwater extraction during dry months by injecting excess surface water in wet months. The JVWCD desires to receive the permission to add the volume of the injected water to its preexisting water rights. However, the Utah Division of Water Rights (UDWR), which determines water rights for the region, believes not more than 90% of the injected water can be recovered by the same ASR wells, if storage duration is 13 to 24 months. Therefore, the UDWR-assigned additional water right is only 90% of the volume of the injected water for storage duration of 13 to 24 months. The additional water right for storage duration of 25 to 36 months is 80% of the injectate volume and so on. In fact, the proportion of the injected water that is recoverable from the same well is the basis for quantifying the
performance of this ASR system. To date, no studies have evaluated the performance of such an ASR system in a FWA.

To address this need, we define recovery effectiveness (REN) as a performance index of this type of ASR systems in a FWA:

\[
\text{REN} = \frac{V_{E,\text{Inj}}}{V_I}
\]  

\(V_{E,\text{Inj}}\) is the volume of the injectate contained within the extracted water, and \(V_I\) is the volume of the injected water. Equation 2 quantifies the proportion of the injected water that the same ASR well can recover during extraction periods, regardless of the total volume of extracted water.

Figure 2-1- The study area. (a) Location of the JVWCD ASR project in Utah. (b). Generalized diagrams showing the locations of shallow unconfined aquifer and principal aquifer; Modified from Thiros et al. (2010).
As a side note, REN is also applicable for ASR systems in saline aquifers. Although not defined as REN, ASR managers can measure it in the field by plotting the total recovered water volume versus the TDS of the recovered water and then integrating beneath the curve (Pyne 1995, page 103). Equation 3 shows the relation between REN and RE in saline aquifers:

\[
RE_{\text{Saline}} = REN + \frac{V_{E\text{Amb}}}{V_I}
\]

\(V_{E\text{Amb}}\) is the volume of the ambient groundwater contained within the extracted water.

Note that quantifying REN in saline aquifers usually has little importance because as long as the extracted water has acceptable quality for intended purpose, it is not critical to know what portion of the extracted water comes from injected water versus ambient groundwater.

In order to measure REN, the JVWCD tried extensive testing to track recoverable stored water in the aquifer by monitoring concentrations of natural tracers. However, the results were uncertain and provided only general trends (SLCWCD 1996). This necessitates the use of modeling to estimate REN for the JVWCD ASR system.

In this study, we demonstrate a methodology to calculate REN in freshwater aquifers using groundwater flow and transport simulations. We use the MODFLOW (McDonald and Harbaugh 1988) and MT3DMS (Zheng and Wang 1999) models. Lacking appreciable density difference between injected water and native groundwater, there is no need to use density-dependent groundwater models. In addition, in the JVWCD ASR
system, the quality of the recharged water not only is very high, but also is very similar in chemical constituents to the native groundwater. This minimizes the potential for geochemical problems (SLCWCD 1996). Therefore, for a given ASR operational setting (i.e. injection/extraction rates and durations), background seepage velocity \( V_{\text{Seepage}} \) is the predominant factor that can affect REN in the JVWCD ASR system.

\[
V_{\text{Seepage}} = \frac{K \times i}{\text{Porosity}}
\]

(4)

In Equation 4, \( K \) is the hydraulic conductivity of the screened layer, and \( i \) is the background hydraulic gradient (the gradient before beginning the ASR operation). As \( V_{\text{Seepage}} \) increases, more injectate departs the well’s capture zone and less water will be recoverable from the same well, therefore, REN decreases.

Specifically, we want to examine the feasibility of achieving REN more than 90% for the ASR wells with storage duration of 13 months. For an accurate examination, we want to prepare a refined model that is computationally inexpensive, yet 1) provides the most accurate background gradient (\( i \) in Equation 4), and 2) allows examining the effect of screening in different strata—examining different values of \( K \) in Equation 4. To do so, we employ a two-stage grid refinement technique on a USGS-calibrated MODFLOW regional model (Lambert 1995a) to prepare refined local models. The procedure enables considering site-specific hydrogeology and aquifer heterogeneity, the factors that can greatly affect ASR performance (Pavelic et al. 2006; Reese 2002; Guo et al. 2015). The refinement procedure also considers the monthly changes in background
stresses (e.g. pumping from non-ASR wells). These features allow computing an accurate transient flow field. Many previous ASR studies employ hypothetical models, homogeneous aquifer parameters, and constant head boundaries creating a uniform background gradient (Merritt 1986; Lowry and Anderson 2006; Brown 2006). Whereas the aforementioned procedure allows addressing the effects of $i$ and $K$, we perform sensitivity analysis to investigate the effects of porosity (the third factor in Equation 4) on REN.

We present the methodology by implementing it on one of the JVWCD ASR wells named SLC8 (Figure 2-1a) to evaluate the achievable REN for storage duration of 13 months. We also assess the effect of different screen interval schemes for improving REN. Finally, we investigate the degree of importance of vertical heterogeneity on REN in FWAs. To do so, we compare the results of SLC8, which has a low background gradient, with JVWCD ASR well SLC22 located in an area with a steeper gradient.

2-2-Previous Modeling Studies

Lambert (1995a) developed a yearly transient state MODFLOW model to simulate the quaternary-age basin-fill aquifer in Salt Lake Valley using hydrologic data of 1969-91. The study calibrated the model to measured water-level changes and estimated annual gains in the Jordan River. Areally, the model grid is 94 rows by 62 columns, with each cell 563 m on a side. Vertically, the model divides the groundwater system into seven layers. The top two layers represent a shallow unconfined aquifer and
an underlying semi confining unit in the center of the valley (Figure 2-1b). Layers 1 and 2 are absent on the margins of the valley including some parts of the ASR project area.

Layers 3 through 7 represent the principal aquifer, which consists of 1) a confined zone beneath the confining unit, and 2) the deep unconfined zones near the margins of the valley (Figure 2-1b). The JVWCD ASR wells are all screened in the principal aquifer. Layer 3, the uppermost layer of the principal aquifer, is modeled as a "convertible" layer in the MODFLOW model. Figure 2-2 shows the extent of confined and unconfined conditions in layer 3. Most of the JVWCD ASR wells are spatially located in the unconfined area of the principal aquifer. In the ASR project area, the thicknesses of model layers 3 to 7 are 46, 46, 46, 61, and 61 m respectively. The largest source of recharge to the principal aquifer is seepage from the surrounding mountains in the east side of the valley. The principal aquifer gradient is steep near the mountains and flattens toward the valley (UDWR and USGS, 1971). Lambert (1995a) provides more details on model boundaries and calibration.

An advective particle tracking study by the USGS (Lambert 1995b) estimated an effective porosity of 40% for model layers 1 and 2 and an effective porosity of 30% for the principal aquifer (i.e. model layers 3 to 7). Another study by the USGS (Stolp 2007) used the same values of effective porosity in a particle-tracking simulation. Without altering any calibrated aquifer properties obtained by Lambert (1995a), Stolp (2007) updated groundwater withdrawals and recharge values to develop a steady state model representing the average conditions of 1997-2001 in Salt Lake Valley.
2-3- Grid Refinement Techniques

Preparing sufficiently refined models for an accurate estimation of REN is necessary for this water rights negotiation purpose. Higher resolution models allow modeling the ASR well and other neighboring pumping wells close to their actual locations. Furthermore, a transport model usually needs a more refined grid than a flow model for accurate contamination simulation and for limiting numerical instability (Zheng and Bennett 2002, Konikow 2011). Employing globally refined grids and variably spaced grids are two approaches for preparing refined flow models. However, these
methods can provide either computationally intensive models, or models with large numerical errors (i.e. large mass balance errors) (Mehl and Hill 2006).

Two alternative approaches, the telescopic mesh refinement (TMR) (Ward et al. 1987; Leake and Claar 1999) and local grid refinement (LGR) (Mehl and Hill 2006 and 2013) methods, use the heads or flows computed by a “parent” larger model to define the perimeter boundaries for a “child” local-scale model. These two methods are especially beneficial for transport modeling because the mesh is only refined locally in the area of interest, and the rest of the regional model is removed before implementing transport modeling. This significantly decreases the run time of the transport model. Also, models using these methods are less likely to have unacceptable mass balance errors than models using a variably spaced grid. In addition, these methods enable the modeler to systematically examine different horizontal or vertical grid sizes and evaluate their effects on the results.

TMR and LGR methods differ in how a child model couples with a parent model. The TMR technique simply applies computed heads or flows from the parent model as specified perimeter heads or fluxes of the child model, and then the child model runs independently. This “one-way” coupling technique results in some inconsistencies across the interface of parent and child models. However, the LGR technique uses a “two-way” coupling method in which iterative feedbacks continue between the child and parent models until reaching user-specified consistencies at interface.
The LGR procedure begins by simulating the parent model with its entire domain. Head values computed from the parent model are applied as specified head conditions along the child-model perimeter. For subsequent iterations, the parent-model cells covering the domain of the child model are eliminated such that the parent model has a hole at the area of the child model. Specified flux conditions are applied for the parent-model cells along the interface with the child model. The values of these specified flux boundaries are computed by running the child model—after running the child model, the fluxes along the child-model perimeter are calculated and used as the parent-model flux boundary conditions. On the other hand, running the parent model computes the updated specified heads along the child-model perimeter. Iterations update the coupling boundary conditions—specified heads at the local model and specified fluxes at the parent model—until both the head change and the flux change at boundaries are smaller than user-specified criteria. LGR iterations ensure consistency of heads and fluxes between the two models. (Mehl and Hill 2006).

The practical importance of the difference between TMR and LGR techniques is that in implementing the TMR technique, the boundaries of the local model should be sufficiently far from the area of interest in order to minimize the effects of boundaries on the results. Therefore, although implementing the LGR technique is more complex, the LGR technique is superior for making an accurate small domain model needed for a computationally efficient transport run. We use both TMR and LGR techniques in this study, as shown in subsequent sections.
2-4- Methodology

2-4-1- Parent Model Preparation

Because the JVWCD ASR system began operating in 2000, we use the resulting heads obtained from the Stolp (2007) model, which represent the average conditions of 1997-2001, as the initial conditions before ASR operation. To model a typical ASR operation, we prepare a 21-month transient model and employ the aquifer parameters calibrated by Lambert (1995a). We acquire the monthly values of model stresses (e.g. pumping of background supply wells, evapotranspiration (ET), and precipitations in the mountains and valley) using the best estimate of these data in the region. For evapotranspiration, only the maximum ET flux (EVTR in MODFLOW EVT package) can differ for each period of the monthly model.

Based on the data obtained from JVWCD, we assume monthly operation in the SLC8 well as shown in Table 2-1. The volumes of injection and extraction are 343,000 and 660,000 m³ respectively. Extraction volume is more than injection volume because of the preexisting water rights in this well before the ASR project. Periods 1 to 3 represent the months January to March before injection in the ASR well. Injection occurs from period 4 (April) to period 6 (June), and extraction occurs in periods 20 and 21 (Months August and September of the following year). Periods 7 to 19 represent storage duration of 13 months.
Table 2-1-ASR operation for SLC8

<table>
<thead>
<tr>
<th>Period</th>
<th>Month</th>
<th>Injection rate (m$^3$/d)</th>
<th>Extraction rate (m$^3$/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 to 3</td>
<td>Jan to Mar</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4 to 6</td>
<td>Apr to Jun</td>
<td>1640, 4890, 4890</td>
<td>0</td>
</tr>
<tr>
<td>7 to 19</td>
<td>Jul to next year's Aug</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>20 and 21</td>
<td>Next year's Aug and Sep</td>
<td>0</td>
<td>11000, 11000</td>
</tr>
</tbody>
</table>

2-4-2- Local Flow Model Preparation

As mentioned before, to make a small domain refined model needed for a computationally efficient transport run, LGR technique is superior over TMR. However, using one-stage refinement with LGR cannot provide accurate specified heads/fluxes along the boundaries of the local models, if the selected domain contains only a few cells of the parent model. Also, large disparity between cell sizes of parent and child models is not recommended because it increases errors at the boundaries of the child model (Mehl and Hill 2006). In this study, regional model cell size is 563 m by 563m and, as shown later, the most refined model that we create has much smaller cell size of 11.75m by 11.75 m.

For these reasons and considering the importance of background hydraulic gradient for accurately estimating REN, we implement grid refinement in two stages. In the first stage, we apply the TMR technique to the regional model to prepare a “TMR
model” having boundaries far enough from the ASR well. The child TMR model has uniform cell size of 47m, which is one twelfth of regional model cell size. Then, we implement the LGR technique on the TMR model for the area around the ASR well to prepare “LGR models” with different horizontal and vertical cell sizes. Figure 2-2 shows the areal extents of the TMR and LGR models within regional model layer 3. All the refined models (TMR and LGR models) only simulate the principal aquifer. Figure 2-3 shows the vertical layers at the location of SLC8 well in regional, TMR, and LGR models.

Figure 2-3-Vertical discretization in different models used for SLC8 well. (a) Regional model. (b) TMR model and LGR models without vertical refinement. (c) Vertically refined LGR model
We prepare four different LGR models from the TMR model (Table 2-2). To evaluate the effect of model horizontal grid size on computed REN, we prepare three LGR models with the same domain (as shown in Figure 2-2) but with different horizontal grid sizes. For the 1st through the 3rd LGR models, the grid sizes are one-half, one-third, and one-fourth of the TMR model cell, respectively. We use ModelMuse (Winston 2009), a free MODFLOW graphical user interface from USGS, to prepare refined mesh input files of LGR models from the TMR model. We use the MODFLOW-LGR2 code (Mehl and Hill 2013) to prepare accurate specified head boundaries (after performing the LGR iterations) for LGR models.

Although preliminary simulations revealed that for a given hydrogeological setting, vertical refinement does not affect REN estimation, we prepare the 4th LGR model with a 11.75m horizontal grid size but also with refined vertical layers (Figure 2-3). The vertically refined 4th LGR model will more accurately evaluate the vertical distribution of injected water during ASR operation. We do not apply vertical refinement in layer 1 of the TMR model because a thick upper layer prevents simulating dry cells in the unconfined part of the principal aquifer. The SLC8 well is open within layers 6 and 7 of the regional model, which is the deepest part of the principal aquifer. Vertically refined LGR model results from refining TMR model layers 2 and 3 (regional model layers 4 and 5) to four sublayers and refining TMR model layers 4 and 5 (regional model layers 6 and 7) to five sublayers. This provides almost similar thicknesses for layers 2 to
19 of the vertically refined LGR model. Table 2-2 summarizes the refined models created to analyze ASR operation in well SLC8.

<table>
<thead>
<tr>
<th>Description</th>
<th>Horizontal cell size (m)</th>
<th>Vertical refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMR model</td>
<td>47</td>
<td>No</td>
</tr>
<tr>
<td>1st LGR model</td>
<td>23.5</td>
<td>No</td>
</tr>
<tr>
<td>2nd LGR model</td>
<td>15.7</td>
<td>No</td>
</tr>
<tr>
<td>3rd LGR model</td>
<td>11.75</td>
<td>No</td>
</tr>
<tr>
<td>4th LGR model</td>
<td>11.75</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Refined models have monthly periods and consider the monthly effect of the background stresses that are within their domains. Specified boundaries along the borders of the refined models are also monthly transient. For each period, the specified boundaries are derived from the corresponding period of the regional model using the TMR or LGR techniques. For the boundaries of the TMR model, we use transient specified fluxes. This facilitates investigating the accuracy of TMR implementation. For the boundaries of the LGR models, as mentioned, the MODFLOW-LGR2 code uses transient specified heads. In preparing refined models, we retain all physical properties from the calibrated regional model. Also, we use the revised multi-node well (MNW2) package (Konikow et al. 2009) in refined models to simulate the multinode ASR well.
The two-stage refinement method provides sufficiently refined models with small domains while providing accurate specified boundaries. The specified boundaries impose the background gradient at the ASR well. Appendix A presents more details about the implementations of TMR and LGR techniques in this study.

2-4-3- Transport Modeling

Transport modeling is an imperative part of evaluating performance of ASR systems. We employ transport modeling on the refined flow models to estimate REN. Because both native groundwater and injected water are freshwater of similar quality, we assume the injected water has an imaginary non-reactive contamination with an arbitrary concentration of 100ppm to distinguish it from native groundwater. We model injection of this “contamination” into an uncontaminated freshwater aquifer with background concentration of zero. Transport modeling determines blending of injected “contamination” with the native groundwater and tracks the movement of the injected “contamination” during ASR operation. The estimated REN (Equation 2) equals the percent of the injected "contamination" that the same ASR well can recover.

We use the MT3DMS code with the total variation diminishing (TVD) explicit finite difference solution technique to minimize numerical dispersion. We assume effective porosity of 0.3 for all cells in the refined models based on two USGS studies which used porosity of 0.3 for the principal aquifer (Lambert 1995b and Stolp 2007). In each flow time step, MT3DMS calculates and uses an optimal transport step size which
meets the various stability criteria. In order to provide results free from oscillation, we use the Courant number of 0.5 for all simulations. The Courant number represents the number of cells a particle is allowed to move in any direction in one transport step. MT3DMS determines the transport step sizes to ensure achieving this Courant number (Zheng and Wang 1999). We use ModelMuse (Winston 2009) to prepare input files needed for MT3DMS run.

We do not use the reaction package of MT3DMS because both injected and native groundwater are essentially freshwater of similar quality. However, we need to utilize both advection and dispersion packages in our transport modeling. Inclusion of the dispersion package is necessary to accurately quantify REN, because it will never be practical to accurately define the velocity field by only using the results of the flow models. Neglecting dispersion in transport modeling unrealistically overestimates the performance of ASR systems (Lowry and Anderson 2006).

2-4-4- Dispersivity Values

Estimating dispersivity values is one of the challenges in transport modeling (Konikow 2011). Dispersivity is a physical parameter that reflects the nature of the aquifer’s heterogeneity. The more one can represent the aquifer’s heterogeneity in the flow model, the smaller values of dispersivity is needed in the transport model— if flow model heterogeneity were fully detailed in the flow model, most solute spreading could be represented by advection and, therefore, very small dispersivity values (i.e.
laboratory or small scale values) would be needed. Davis (1986) shows that a dispersivity value as low as 0.01m can be used with a flow model having detailed heterogeneity to reproduce an observed 500m long solute plume.

The impracticality of representing a detailed heterogeneity within a flow model, however, forces modelers to use large values of dispersivity to achieve a reasonable match during calibration (Freeze and Cherry 1979; Frind and Hokkanen 1987; Konikow 2011). That impracticality also results in obtaining longitudinal dispersivity values which generally depend on measurement scale (Gelhar 1992, Schulze-Makuch 2005, and Xu and Eckstein 1995).

In this study, due to lack of observation data to calibrate for the dispersivity value, we estimate dispersivity based on the scale of measurement. For this ASR well, the scale equals the maximum probable injectate plume length. We compute the scale by summing two terms:

1) The radius of the theoretical ASR bubble at the end of the injection period

2) The estimated travel distance of the injectate during 13 months of storage time (estimated by multiplying the seepage velocity by the storage duration)

For SLC8, we sum the two above terms for both regional model layers 6 and 7, and use the larger value as the scale of the problem. Using the estimated scale within the formula of Xu and Eckstein (1995) provides the dispersivity value of 4.5m. We consider 4.5m a conservative estimate for analyzing the feasibility of obtaining a REN exceeding 90%. Our methodology theoretically needs lower values of dispersivity than
does a semi-equivalent homogenous model with uniform boundaries. This occurs because our methodology preserves the horizontal and vertical heterogeneity and uses transient boundaries (to simulate the velocity field more accurately). We also assume horizontal and vertical transverse dispersivities one and two orders of magnitude smaller than longitudinal dispersivity, respectively.

2-5- Results

2-5-1- Accuracy of TMR and LGR Models

In the TMR technique, after updating the local model with higher resolution data (herein we only improve the location of ASR well and other background pumping wells) and running the local model, there might be some inconsistencies at the interface of the local and parent models. In preparing the TMR model, we assigned specified flows obtained from the regional model along the perimeter of the TMR model. Therefore, comparison of the computed heads in the boundaries of the TMR model with corresponding heads in the regional model provides a measure of consistency between the two models.

For example, Figure 2-4a shows the head differences at the boundaries of the TMR model (TMR model heads minus regional model heads) in period 20 using a box-and-whisker plot. Period 20 has the highest head differences between the two models because this period is the first period that imposes the highest stress on the system (through the extraction rate of 11000m3/d). Therefore, we investigate the accuracy of
TMR and LGR techniques at this period. In this figure, the box shows the middle 50% of data, and the thicker line inside the box shows the median. The whiskers are the two lines outside the box that extend to the highest and lowest data excluding the outliers. Outliers are individual points beyond the whiskers. The head difference in most boundary cells is within the box and whiskers in the range of -0.25 to +0.5m. This difference is acceptable because the boundaries of the TMR model are far from the ASR well. Because TMR is a one-way coupling technique, there is no formal way to improve consistency between the two models.

On the other hand, the LGR technique can decrease the inconsistency between parent and child models by iteratively adjusting heads and fluxes across the interfacing boundary of the two models. In this study, LGR adjusts these boundary conditions using the average values of the current and previous iterations. For example, Figure 2-4b shows that the MODFLOW-LGR2 code needs six iterations in period 20 to reduce the maximum head difference (LGR model heads minus TMR model heads) at boundaries of an LGR model from 0.3m to our 0.01m goal.

Note that the first iteration of the LGR technique is equivalent to the one-way coupling in the TMR technique. Comparing the results of the TMR model (Figure 2-4a) with the maximum head difference for the first LGR iteration (i.e. 0.3m) shows that the absolute values of head differences in many boundary cells in TMR model are larger than 0.3m. This occurs because the change in cell sizes between the regional model and the TMR model is much larger than the change in cell sizes between the TMR model and
LGR models. This shows the benefit of employing two-stage refinement to achieve accurate local models where there is a large disparity between cell sizes of the parent and child models.

2-5-2-Effects of Horizontal Grid Size

After preparing refined local models, we conduct transport modeling to estimate REN. For the assumed ASR operation for SLC8 (Table 2-1), we implement transport modeling using TMR model and the 1st, 2nd, and 3rd LGR models (Table 2-2). For this section, we assume the SLC8 well is fully screened across regional model layers 6 and 7.

Figure 2-4- Accuracy evaluation of refinement techniques. (a) A boxplot showing TMR accuracy; (b) A typical MODFLOW-LGR2 code iteration to improve the consistency between TMR and LGR models
Figure 2-5 shows SLC8 REN estimation for storage duration of 13 months using different refined models. The figure re-emphasizes the importance of model cell sizes in transport simulations. The refined model with a cell size of 11.75m proves the feasibility of achieving an REN of more than 90%, while the refined model with a cell size of 47m proves the opposite. Note that this effect is only due to improvement in accuracy of numerical modeling—no attempt was done to improve the heterogeneity of the flow model in more refined models. As shown by the regression line, there is almost a linear relation between model grid size and REN. Figure 2-5 suggests preparing transport models with grid spacing as small as possible but not larger than 15m (50ft) for a reasonable estimation of REN (in FWAs) or \( R_{\text{Saline}} \) (in saline aquifers). The refinement technique presented in this study allows preparing sufficiently refined models from larger scale models. It is worthwhile to mention that using the regional model (with cell size of 563m) in a transport model provides unreasonable results with very low REN (less than 5%) for SLC8.

![Figure 2-5-The impact of model horizontal discretization on REN](image-url)
The 3rd and 4th LGR models (see Table 2-2) provide identical results. This is consistent with the preliminary simulations showing that for a given hydrogeological setting, vertical refinement does not affect REN.

2-5-3- Sensitivity Analysis on Aquifer Parameters

Using the 3rd LGR model and assuming the specified heads along the boundaries remain unchanged, doubling or halving the horizontal hydraulic conductivity of the model’s cells (or doubling or halving the background seepage velocity) changes REN from 94.5% to 93% or 95.5%, respectively. The effects are small because although the velocity is doubled, it is still such low that it can provide a high REN. This occurs because the well’s low background gradient (i=0.0007) dominantly keeps the seepage velocity low (Equation 4), making the results insensitive to conductivity changes. For the same reason, the REN is relatively insensitive to porosity changes (REN ranges 3% for porosity ranging from 0.2 to 0.4). However, increasing the hydraulic conductivity 3 times reduces REN to less than 90% (88.4%). Increasing the hydraulic conductivity 5 and 10 times reduces REN to 77% and 43%, respectively. Changing dispersivity by 50% (ranging from 2.25 to 6.75m) causes a 2% range in REN. Possibly, factors other than low velocity affect REN insensitivity to dispersivity. Supplementary analyses also show that REN is generally insensitive to changes in the storativity of a confined aquifer.
2-5-4- Analyzing the Vertical Distribution of Injected Water

Before investigating the effects of different screen interval schemes on achievable REN, it is beneficial to analyze the vertical distribution of injected water during an ASR operation. To improve the accuracy of observations for SLC8, we use the vertically refined LGR model (4th LGR model in Table 2-2) with 19 layers. We modified the MT3DMS source code to report remaining injectate in each layer for each period. Figure 2-6 shows the vertical distribution of injectate for a fully screened interval across regional model layers 6 and 7 (layers 10 to 19 of the 4th LGR model) at the end of injection (period 6), during storage duration (periods 7-19), and at the end of extraction (period 21) in SLC8. The regional model layer 6 (LGR model layers 10 to 14) is six times more permeable than regional model layer 7 (LGR model layers 15 to 19). Therefore, LGR model layers 10 to 14 accept almost six times more injectate than layers 15 to 19 during injection.

Figure 2-6 shows that the amount of injectate in each layer does not change during storage time (periods 7 to 19) and is the same as the end of injection (period 6). This occurs because in the absence of pumping, the relative heads of different layers remain constant and no vertical hydraulic gradient is induced between layers. During injection, while head increase in screened layers induces horizontal flows in those layers, vertical hydraulic gradient also induces vertical transport to neighboring non-screened layers. This vertical gradient causes layer 9 to receive almost 4% of total injected water. Although layer 9 receives a small amount of injectate during injection, it
retains a high proportion (18%) of the final non-captured injectate. Note that this observation occurs because of the high recovery of injected water (REN=94.5%) through screened layers in SLC8 well. The existence of a high proportion of unrecovered injectate in unscreened layers will not usually occur for wells having low REN—in low-REN wells, most unrecovered injectate is in screened layers.

Figure 2-6-Vertical distribution of ratio of remaining injectate to total injectate volume during ASR operation of SLC8 when modeled using a fully screened interval across LGR model layers 10 to 19.
2-5-5- Effect of Different Screen Intervals Schemes

This section evaluates the effect of different screen interval schemes on REN in SLC8. Again, to improve the accuracy of observations, we use the vertically refined LGR model. To examine the effect of different screen intervals on the final remaining injectate (in period 21), Figure 2-7 contrasts the results shown in Figure 2-6 (here we call it Scheme A) with the results of three other screen schemes. The MNW2 package allows the easy examination of different well screen intervals. Schemes B, C, and D assume fully screened across regional model layer 6 (LGR model layers 10 to 14), fully screened across regional model layer 7 (LGR model layers 15 to 19), and the actual screen interval based on well logs of the ASR well, respectively. Mapping the actual well log on the LGR model shows that the ASR well is open in layers 10 to 14 and 17 to 19 of the LGR model.

Comparing Scheme A with Scheme D shows again the effect of trapping some of the injected water in non-screened layers (i.e. in layers 15 and 16 in Scheme D) which resulted in 1.1% decrease in REN for Scheme D. Scheme C achieves the highest REN. This occurs because of two reasons. First, it is the only scheme that is not screened in the higher permeability layer 6. Injected water in the higher permeability layer has higher seepage velocity (Equation 4) causing movement further downstream of the well and reducing the well’s capability to recapture it. Therefore, the higher the hydraulic conductivity of the screened layer, the less REN is achievable from that layer. Second, Scheme C allows the least possibility of injectate transport to non-screened layers because the bottom of this screen scheme is impermeable bedrock. Conversely, Scheme
D yields the lowest REN because while it is open in higher permeability stratum, it also provides some non-screen layers between screened layers.

In order to achieve a higher REN, the results suggest using screen intervals in strata with lower permeability as long as it does not hamper the functionality of the ASR well. Screening the ASR wells in strata with too low permeability will result in clogging during injection and low yield during extraction. To further improve the REN for the wells with already high REN (e.g. SLC8 well), using a continuous screen interval can slightly increase the REN. In addition, it is generally recommended to avoid screening in shallow and/or thin strata. Using very thin screen intervals can increase clogging (which decreases recharge efficiency), and screening in shallow layers can cause excessive groundwater mounding (Pyne 1995, section 4-2).

2-5-6- Effect of Vertical Heterogeneity In the Presence of Significant Background Gradient

The results in the previous section suggest that screening in lower permeability layers can improve REN in ASR systems in FWAs. However, the differences in REN between the four analyzed schemes are not considerable. That might imply that vertical heterogeneity is not a pivotal factor in ASR systems in FWAs. This section investigates that conjecture.
Figure 2-7: Vertical distribution of the ratio of remaining injectate to total injectate volume at the end of extraction (Period21) for alternative model representations of Well SLC8: (A) Fully screened across LGR model layers 10 to 19; (B) Fully screened across LGR model layers 10 to 14; (C) Fully screened across LGR model layers 15 to 19; (D) Actual screen intervals.
For ASR systems in saline aquifers, it is well known that vertical heterogeneity can be a crucial factor because of the density contrast between injected water and native groundwater. Maliva et al. (2006) and Guo et al. (2015) show that vertical heterogeneity can cause failure of ASR projects in saline aquifers. To improve RE_{Saline}, Miotlinski et al. (2014) use a partially penetrating screen and complete an ASR well at shallower depths of a saline aquifer. Their intent is to avoid high permeability material in the lower part of the aquifer. On the other hand, Vacher et al. (2006) and Maliva et al. (2006) state that in the absence of density effects (e.g. ASR wells in FWAs), there is virtually no difference in performance of ASR systems in homogenous versus heterogeneous flow zones. Ward et al. (2008) also conclude that “in the density-invariant models there was no significant change in RE with the level of heterogeneity.”

The findings reported by these studies, however, are based on assuming negligible background gradient in their models.

Herein, we assess the importance degree of vertical heterogeneity on REN in the presence of considerable background gradient. To do so, we compare the results of SLC8, which has a low background gradient of 0.0007, with another JVWCD ASR well named SLC22. SLC22 is located closer to the eastern margin of Salt Lake Valley in an area having a steeper hydraulic gradient of 0.0038. We implement the same refinement techniques on SLC22 to prepare a vertically refined LGR model. For consistency, we prepare this model with the same cell size (11.75m) as the 4th LGR model prepared for SLC8. Also, we assume the same monthly ASR operation for SLC22 (Table 2-1). Applying
the Xu and Eckstein (1995) formula yields a higher 6m longitudinal dispersivity value. Injectate advective movement (i.e. the second term for estimating the injectate plume length) is higher at this well than at SLC8 because of the higher SLC22 gradient. SLC22 is screened in layers 4 and 5 of the regional model where layer 4 is only two times more permeable than layer 5. We examine three screen interval schemes for this well: 1) Fully screened across both layers 4 and 5; 2) Fully screened across layer 4; and 3) Fully screened across layer 5. Figure 2-8 shows REN for these three screen schemes for SLC22 and screen schemes A to C for SLC8.

Unlike SLC8, vertical heterogeneity (i.e. different screen interval schemes) has a significant impact on achievable REN for SLC22. If screened only in layer 4, the SLC22 well REN is 3%, whereas if screened only in layer 5, REN is 45.7%. Even screening in both layers provides very poor REN of 5% — Even layer 5 provides much less REN compared to the case of screening only in layer 5. This occurs because in ASR systems in freshwater aquifers, for a given ratio of extraction to injection, a decrease in injection volume decreases REN (Forghani and Peralta 2017b). Therefore, in the case of screening in both layers 4 and 5 because only one-third of the injectate goes to layer 5 (because its transmissivity is half of transmissivity in layer 4) this layer achieves a poorer REN compared to the case of screening only in layer 5. Results in Figure 2-8 demonstrates that for the wells completed in multiple strata, higher permeability layers control the achievable REN.
In summary, whereas Figure 2-7 shows that it is slightly advantageous to have screen intervals in low permeability layers (providing it does not hamper ASR well functionality), Figure 2-8 displays that this beneficial effect increases as the background gradient increases. The very low SLC8 background gradient causes a low seepage velocity (Equation 4) and a high REN, making the effects of hydraulic conductivity of different screened layers insignificant. The same concept explains REN insensitivity to changes in porosity for SLC8. For SLC22, however, seepage velocity and consequently REN are much more sensitive to changes in hydraulic conductivity of the screened layers—background gradient is not the dominant factor controlling REN. Thus, vertical heterogeneity can significantly impact REN for ASR wells located in high gradient areas. In fact, Figure 2-8 shows that the sensitivity of SLC22 to changes in velocity is greater than that of SLC8. Note that the SLC22 REN is also more sensitive than the SLC8 REN to changes in porosity. For the condition of screening across layer 5, REN changes from 30% to 55% for porosities of 0.2 to 0.4. Nevertheless, similar to SLC8, the REN of SLC22 is relatively insensitive to ± 50% changes in dispersivity (i.e. in the range of 3 to 9m). Again, REN is insensitive to changes in confined aquifer storativity.

2-6- Conclusions

For an ASR system developed for water right purposes in a freshwater aquifer (FWA), we propose the recovery effectiveness (REN) as an index to quantify the system's performance— the proportion of the injected water that the same ASR well
can recapture during subsequent extraction periods. Using imaginary contamination to distinguish the injected water from the native groundwater, we present a methodology to quantify REN using transport modeling.

Among other factors, accurate REN estimation needs: 1) considering site specific hydrogeology and aquifer heterogeneity; and 2) employing sufficiently refined models. To satisfy these criteria, we employ a two-stage refinement technique using publicly available codes. The study presents the salient considerations of the refinement technique and displays the advantage of the LGR method to improve the consistency between the parent and local models.
The study shows that preparing sufficiently refined models is essential in REN estimation. Using more horizontally-refined models improves (increases) REN almost linearly in the tested range. Preparing horizontally refined models is especially important if transport model results provide the basis for determining ASR system performance. The presented refinement technique provides an accurate local model with cell sizes 48 times smaller than the original model.

Background seepage velocity, the seepage velocity before beginning ASR operation, is the main criterion affecting REN in the studied ASR system. Accordingly, the study’s results show that screening in less permeable layers, as long as it does not hamper the functionality of the ASR well during injection and extraction (i.e. the well can provide the desired injection/extraction rates), can improve REN. The study further demonstrates that as the background hydraulic gradient increases, the importance of avoiding screening in higher permeability layers increases. In other words, whereas for the wells located in low background gradient (e.g. SLC8 well) vertical heterogeneity insignificantly affects REN, the well’s screen design can crucially affect the achievable REN for wells with high background gradient (e.g. SLC22 well).

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CHAPTER 3
INTELLIGENT PERFORMANCE EVALUATION OF AQUIFER STORAGE AND RECOVERY SYSTEMS IN FRESHWATER AQUIFERS

Abstract

We present an artificial neural network (ANN) based software for rapidly predicting the recovery effectiveness (REN) of aquifer storage and recovery (ASR) wells in fresh water aquifers. The REN performance criterion equals the amount of the water injected in an ASR well that is recoverable via the same well during a specified extraction period. The software circumvents the need to prepare and run computationally intensive simulations, by invoking ANN models as surrogate simulators. The paper presents the development of the ANN models and a graphical user interface (GUI) to facilitate using the ANN models and to perform sensitivity analysis. ANN inputs include all factors significantly affecting REN in freshwater aquifers. The software can evaluate REN in any ASR system whose parameters are within the range of parameters used for training the ANNs in this study.

3-1. Introduction

Aquifer storage and recovery (ASR) is the artificial recharge of excess surface water into an aquifer for later withdrawal. An ASR system provides an alternative to storage in surface reservoirs without many of the environmental concerns, evaporation losses, and costs.
Most ASR studies reported in literature address saline aquifers. Recovery efficiency (here termed RE_{Saline}) is commonly used to quantify the performance of the ASR wells in saline aquifers (Equation 1).

\[
RE_{Saline} = \frac{V_E}{V_I} 
\]

Where \( V_E \) is the volume of extracted water with acceptable quality for intended use, and \( V_I \) is the volume of the injected water.

\( RE_{Saline} \) is measurable in the field during ASR operation. The availability of the field data allows simulation model calibration and subsequent use to analyze \( RE_{Saline} \). Significant density difference between injected water and ambient (or native) groundwater requires using variable-density coupled flow and transport models (Pyne 1995, Ward et al., 2009).

Water managers can also implement ASR systems in freshwater aquifers (FWA). The Jordan Valley Water Conservancy District (JVWCD) began an ASR project in a FWA in Utah, USA, in the year 2000. An objective in developing this ASR system is to receive additional water rights for extraction in dry months by injecting excess surface water in wet months. However, Utah Division of Water Rights (UDWR), which determines water rights for the region, defines the performance of this ASR system as the amount of injected water that the same ASR well can recover. This performance is used as the basis to allocate additional water rights for the JVWCD. Thus, for negotiations about water right allocations, it is necessary to compute what percent of the injected water is
recoverable from the same ASR well. To address this, we use recovery effectiveness (REN) (Forghani and Peralta 2017) as the performance criterion for JVWCD ASR system. Equation 2 shows REN which quantifies the proportion of the injected water that the same ASR well can recover:

\[ REN = \frac{V_{E_{Inj}}}{V_I} \]  

(2)

Where \(V_{E_{Inj}}\) is the volume of injectate available in the total extracted water, and \(V_I\) is the volume of injected water. Note that REN shows the amount of the injected water that is recoverable during the extraction period regardless of the total volume of extracted water. Equation 3 shows the relation between REN and RE in saline aquifers:

\[ RE_{Saline} = REN + \frac{V_{E_{Amb}}}{V_I} \]  

(3)

Where \(V_{E_{Amb}}\) is the volume of ambient groundwater available in the extracted water. Pyne (1995, page 103) shows the procedure to quantify REN in ASR systems in saline aquifers, although its value is not usually of interest for ASR managers in saline aquifers.

Contrary to ASR systems in saline aquifers, estimating REN in FWA during an ASR operation in the field is impossible. This results from the similar quality of injected water and native groundwater. Also, using in-field tracking techniques such as tracer tests is uncertain and inaccurate especially for water right negotiations. Therefore, groundwater modeling is inevitable for a reasonable estimation of REN in FWA.
Several analytical equations address the performance of ASR systems. However, their simplifications prevent using them for an accurate estimation of ASR systems' performance. Gelhar and Collins (1971) developed an analytical equation to estimate concentration change during an injection/extraction cycle at a fully penetrating well in a confined aquifer. The relation, however, does not allow storage duration between injection and extraction and therefore, the effect of storage durations on REN cannot be analyzed. Lu et al. (2011) developed a numerical model to estimate performance of ASR systems under various mass transfer parameters. Among other simplifications, they neglected background flow gradients in their study whereas gradient is the most important factor for ASR systems in FWA. Although there are some analytical equations capable of considering background gradients (Sedighi 2003, Javandel et al. 1984), the limitation of these models is their inability to account for dispersion. Neglecting dispersion can unrealistically overestimate the performance of ASR systems (Lowry and Anderson 2006).

Therefore, we consider flow and transport simulation to be essential for accurately quantifying REN in FWA. For that, here we use MODFLOW (McDonald and Harbaugh 1988) and MT3DMS (Zheng and Wang 1999) models. Using MODFLOW-MT3DMS models, however, can be challenging. Preparing MODFLOW-MT3DMS models can be cumbersome, and simulation times can be large. This prevents analyzing and comparing multiple ASR scenarios in a manageable time (Asher et al. 2015).
To overcome this difficulty, we present a software that rapidly estimates REN (Equation 2) without the need to prepare and run MODFLOW-MT3DMS models. As substitute simulators, the software invokes two trained ANN models. ANNs are powerful nonlinear regression techniques that can identify complex relations between input and output data. Many researchers have utilized ANNs in different fields, including water resources (Hsu et al. 1995, Kralisch et al. 2003, Parkin et al. 2007, Adeloye 2009, Maier et al. 2010, Izady et al. 2013). Several studies employ ANNs as surrogate groundwater simulators in optimization models to reduce computational burden (Aly and Peralta 1999, Coppola et 2007, Fayad et al 2012, Peralta et al 2014). No published study, however, reports developing and using ANN models to quantify the performance of ASR wells. Also, most ANNs reported in the literature are developed for a specific area, or even a specific site within an area. Herein, our generalized ANNs can estimate REN for ASR systems in many areas worldwide.

The dataset used to train and verify the ANNs derive from 10,000 MODFLOW-MT3DMS simulations. Inputs (independent variables) for these simulations differ for seven hydrogeological and operational factors potentially impacting REN. These factors are: background gradient, hydraulic conductivity, injection rate, extraction rate, aquifer thickness, porosity, and longitudinal dispersivity. To address the effect of storage duration on achievable REN, we utilize two different sets of MODFLOW-MT3DMS models for two different scenarios of storage duration. One set of MODFLOW-MT3DMS simulations assumes no storage of injected water (i.e. extraction starts immediately
after injection). The other simulations set allows one year storage of injected water (i.e. extraction starts after storing the injected water in aquifer for 12 months). Each of the two sets involves 5,000 MODFLOW-MT3DMS simulations using random values of independent variables generated within reasonable ranges. MODFLOW-MT3DMS simulations outputs are the computed REN values for each 15 days of extraction up to 120 days.

To identify the significant independent variables for use in ANN model development, we perform a correlation analysis using the 5,000 input-output MODFLOW-MT3DMS datasets obtained for each scenario. Analysis also reveals the relative importance of independent variables on REN. Finally, we develop one ANN for each of the two storage duration scenarios, using 5,000 input-output datasets. We use a cross validation technique to develop parsimonious generalized ANN models.

To handle the large number of MODFLOW-MT3DMS simulations needed for this study, we use parallel processing by the message passing interface (MPI) technique (Gropp et al. 2014). MPI allows running a large number of simulations in parallel on a cluster of computing nodes.

The developed ANNs are alternatives to implementing MODFLOW-MT3DMS simulations to estimate REN in FWA. Using the developed ANNs, one can easily investigate achievable REN for multiple hydrogeological settings or operational factors. This significantly improves the capability to identify ASR optimal locations and operational injection/extraction factors.
3-2. Artificial neural network theory

An ANN works as a universal approximator for complex functional relationships between input and output datasets. There is no need to know or speculate the relation between inputs and outputs as, for example, is needed for the multiple linear regression. The input-output datasets needed for training ANNs can be obtained using field (or observation) data, or simulation model results.

Among many ANN structures proposed and used since the 1950s, three-layer feedforward neural networks are the most popular. Hornick et al. (1989) show that three-layer feedforward ANNs can be trained to model any piecewise continuous function. Figure 3-1 shows an example of a three-layer feedforward ANN. Each layer consists of processing elements called neurons or nodes. The first layer (or input layer) and the last layer (or output layer) consist of input and output data, respectively. The numbers of nodes in these layers are the same as the numbers of inputs and outputs to the ANN model. The middle layer is called the hidden layer. Generally, the number of nodes in the hidden layer is a design issue based upon problem complexity (Govindaraju 2000). Usually, neural networks contain some additional nodes called "bias" (with values equal to one). The bias nodes are analogous to the intercept in a linear regression model and can significantly improve ANN flexibility.

The above ANN structure is termed "feedforward" because information transfers only from a previous layer to the next layer. All the nodes (including bias) from the previous layer are connected to all the nodes of the next layer. Each connection has an
Figure 3-1. An example of a neural network with two input nodes (X1 and X2), two output nodes (Y1 and Y2) and one hidden layer consisting of three hidden nodes associated weight that represents the connection importance. The value of each node in the hidden layer is computed by applying an activation function (usually a nonlinear function) on the sum of the products of the values of input layer nodes and their associated weights (Equation 4). Similarly, the value of each node in output layer is computed by applying an activation function (usually a linear function) on the sum of the products of the values of the hidden layer nodes and their associated weights (Equation 5). Equations 4 and 5 show, respectively, the calculation of the values of one hidden node (H1) and one output node (Y1) in Figure 3-1 by applying a logistic sigmoid function for the hidden layer and a linear activation function for the output layer.

\[
H_1 = \frac{1}{1 + \exp[-(1 \times W_{01} + X_1 \times W_{11} + X_2 \times W_{21})]}
\] (4)
\[ Y_1 = (1 \times W'_{01}) + (H1 \times W'_{11}) + (H2 \times W'_{21}) + (H3 \times W'_{31}) \quad (5) \]

Training, or in other words calibration, of an ANN model involves entering an input-output dataset to the ANN model and optimizing the network weights to minimize the sum of squared of model residuals (residuals are the differences between observed outputs and the predicted outputs by ANN model). Random values are initially assumed for all weights and then learning algorithms are employed to optimize the weights. Among the learning algorithms, the back-propagation algorithm (Rumelhart et al. 1986) is the most popular for training feedforward ANNs.

As mentioned, the number of nodes in the ANN hidden layer strongly affects ANN accuracy. Considering too few hidden nodes prevents adequate representation of model complexity. Considering too many hidden nodes results in "overfitting", which actually provides a model with poor generalization. To illustrate overfitting, we should note that any input-output dataset contains a pattern (or signal) and also some random noises. By developing ANN models, we are interested in modeling only the pattern of the data which actually shows the relations between inputs and outputs. Using too many hidden nodes during training causes the ANN to recognize the noise of the training dataset as well as its pattern. Because the noises are random and change in each dataset, using an overfitted ANN model for predicting other datasets will produce poor results. One method to avoid overfitting is cross validation (Kuhn and Johnson 2013, chp 4). Subsequent sections present the application of the cross validation technique used in this study.
In summary, developing an ANN model using a three-layer feedforward structure involves 1) selecting appropriate activation functions for hidden and output layers; 2) choosing an appropriate learning algorithm to optimize weights; 3) determining the number of nodes in the hidden layer by cross validation; and 4) optimizing and recording a set of weights as the main outcome of an ANN development. To use the developed ANN for predicting new scenarios, one can apply the weights in equations similar to Equations 4 and 5 to estimate the model response to new input data.

3-3. Methodology

3-3-1. Independent variables selection

To prepare the ANN models capable of predicting REN for desired hydrogeological or operational settings, we need to consider all the factors that can impact REN. Herein, we consider seven factors as potentially significant independent variables for REN estimation. These factors are: 1) Background gradient; 2) Hydraulic conductivity; 3) Injection rate; 4) Extraction rate; 5) Aquifer thickness; 6) Porosity; and 7) Longitudinal dispersivity. We select these factors based on previous ASR studies (Merritt 1986, Pyne 1995, and Lowry and Anderson 2006), as well as preliminary MODFLOW-MT3DMS simulations implemented in this study.

The preliminary analyses show that for the same value of transmissivity, which for a confined aquifer is calculated as the product of hydraulic conductivity (K) and aquifer thickness (b), different combinations of b and K provide different REN results.
This necessitates using $K$ and $b$ explicitly instead of using a transmissivity value as an independent variable. Also, preliminary analyses show that computed REN is insensitive to the value of specific storage (for a confined aquifer); so we do not use the storativity value as an independent variable and therefore we assume a constant specific storage (equals to 1E-6) for all simulations.

3-3-2. Ranges of independent variables

Table 3-1 shows the range of independent variables considered in this study. The only difference in the range of independent variables between the two storage duration scenarios is related to the upper limit for the gradient value. MODFLOW-MT3DMS simulations revealed that for Scenario 2 (storage duration of 1 year), background gradients more than 0.004 produce negligible REN regardless of the values of other factors. Therefore, we consider the upper limit of the gradient for Scenario 2 as 0.004. Note that limiting the gradient's upper limit to the value of 0.004 is not problematic for the wells with gradient more than 0.004 (e.g. wells SLCWCD3 and SLCWCD28 in Table 1-1) because any gradient value greater than 0.004 results in a similar negligible REN (less than 5%). To be more precise, for the wells with gradient more than 0.004, the developed ANNs can estimate the maximum achievable REN (which will be an insignificant value) by applying the gradient value of 0.004.
Table 3-1. Ranges of independent variables values

<table>
<thead>
<tr>
<th>Independent variable</th>
<th>Range (Metric)</th>
<th>Range (US Units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gradient</td>
<td>0 to 0.015 (No storage duration)</td>
<td>0 to 0.015 (No storage duration)</td>
</tr>
<tr>
<td></td>
<td>0 to 0.004 (1 year storage)</td>
<td>0 to 0.004 (1 year storage)</td>
</tr>
<tr>
<td>Hydraulic conductivity (K)</td>
<td>13 to 70 (m/d)</td>
<td>43 to 230 (ft/d)</td>
</tr>
<tr>
<td>Injection rate</td>
<td>1225 to 9785 (m³/d)</td>
<td>0.5 to 4 (cfs)</td>
</tr>
<tr>
<td>Ratio of Ext/Inj rate</td>
<td>1 to 3</td>
<td>1 to 3</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.1 to 0.5</td>
<td>0.1 to 0.5</td>
</tr>
<tr>
<td>Longitudinal dispersivity</td>
<td>1.5 to 15 (m)</td>
<td>5 to 50 (ft)</td>
</tr>
<tr>
<td>Aquifer thickness (b)</td>
<td>15 to 150 (m)</td>
<td>50 to 500 (ft)</td>
</tr>
</tbody>
</table>

Also, of interest is the range selected for hydraulic conductivity (K). We use 70 m/d (230 ft/d) as the conceptual upper limit of hydraulic conductivity for unconsolidated basinfill materials (Lambert 1995, page 15). We initially assumed 7 m/d as the lower limit of K to be one order of magnitude smaller than the assumed upper limit. However, preliminary modeling results showed that using a K value this low produces large head fluctuations at the well during ASR operation which also can result in a dry cell. This might imply that it is not operationally appropriate to have an ASR well in a fresh water aquifer with hydraulic conductivity this low. So, we increased the lower limit of K values to 13 m/d (43 ft/d).

The lower limit of 13 m/d for K values is insufficient for some of the JVWCD ASR wells as shown in Table 1-1. Therefore, the developed ANNs will have a limitation to accurately estimate REN for these wells. For these wells, however, the developed ANNs can estimate the minimum achievable REN by applying the hydraulic conductivity value of 13 m/d.
We model extraction rate values by multiplying the injection rate by the ratio of extraction to injection rate. We assign values greater than one for the ratio of extraction rate to injection rate. ASR wells in freshwater aquifers usually have a preexisting water right associated with the time before converting to an ASR well (and enabling injection to them). Therefore, we do not consider extraction rates lower than injection rates in this study.

The assumed range of longitudinal dispersivity values is from 1.5 to 15m. The upper limit of 15m results from using the maximum probable injectate plume length within the formula of Xu and Eckstein (1995). We assume horizontal and vertical transverse dispersivities one and two orders of magnitude smaller than longitudinal dispersivity, respectively. Also, we assume the effect of molecular diffusion is unimportant in this study.

3-3-3. The MODFLOW-MT3DMS models

We use MODFLOW-MT3DMS simulations to prepare the input-output dataset needed for training the ANN models. We construct two different MODFLOW-MT3DMS models to address two storage duration scenarios. For each scenario, we implement 5,000 MODFLOW-MT3DMS simulations by randomly changing the seven independent variables within their Table 3-1 ranges.

For both scenarios, we model a fully penetrating ASR well in a homogenous one-layer confined aquifer. We assume constant-head boundaries on the eastern and
western edges of the model, and assume the ASR well is at the center of the model area (Figure 3-2). We assume no-flow boundary conditions on the northern and southern edges of the model, which means water cannot enter or leave the model through these boundaries. The model domain is 10,000m by 10,000m and is discretized uniformly to cells of 10m by 10m (creating 1,000 rows and 1,000 columns). We use such a large domain to ensure the validity of the assumption of constant-head boundaries during ASR operation. However, to reduce the run time of the transport model, we make the cells that are very far from the ASR well inactive in MT3DMS model. Selecting cell sizes of 10m can give acceptable accuracy in REN estimation without making the computational demands of transport models too expensive. Aquifer top elevation is invariably zero meters while bottom elevation changes (and takes negative values) to create models with different aquifer thickness in the range shown in Table 3-1.

The background gradient is from the eastern side to the western side of the model. We assume the specified head on the western boundary constant and equal to 330m. For the eastern boundary, the specified head values change in the range of 330 to 480m for Scenario 1 (to induce gradients of 0 to 0.015) and in the range of 330 to 370m for Scenario 2 (to induce gradients of 0 to 0.004). We assume the minimum constant head boundaries as 330m to ensure that for all conditions of independent variables, the calculated head at the well is above the top of aquifer (zero meters) and the aquifer truly remains as confined.
For both scenarios, we assume two months of injection presumably in two months of spring. This is a reasonable estimate of the duration of injection for many ASR systems. We use a uniform injection rate for two months of injection. Also, we assume extraction duration to be 4 months. Again, we use a uniform extraction rate in 4 months of extraction era.

For Scenario 1 models, we use seven monthly stress periods, each with two time steps. The first stress period models the steady state conditions before ASR operation to induce the desired background gradient. Injection occurs in periods 2 and 3, while extraction occurs in periods 4 to 7. For Scenario 2 models, we use 19 monthly stress periods, each with two time steps. Again, the first stress period represents the steady state conditions before ASR operation to induce the desired background gradient. Also, injection occurs in periods 2 and 3. No pumping occurs in periods 4 to 15 to allow
storage of injected water for 12 months. Then, extraction occurs for 4 months in periods 16 to 19.

Because both native groundwater and injected water are freshwaters of similar quality, in MT3DMS model we assume injected water has 100 ppm of imaginary non-reactive contaminant, to distinguish it from uncontaminated native groundwater. MT3DMS tracks the injected "contamination" during ASR operation and computes the amount of the injected "contamination" that the same ASR well recovers. The estimated REN (Equation 2) equals the ratio of "contamination" extracted by the ASR well divided by the total injected "contamination".

We use both advection and dispersion packages of the MT3DMS model. Using the dispersion package is essential to accurately estimate REN (Lowry and Anderson 2006). However, we do not need the reaction package because both injected water and native groundwater are actually freshwaters of similar quality. As the solution method in MT3DMS, we use the total variation diminishing (TVD) explicit finite difference technique to minimize numerical dispersion.

The results of MT3DMS simulations allow calculating cumulative REN at each time during extraction. Here, we record eight REN values after 15, 30, 45, 60, 75, 90, 105, and 120 days of extraction, and call them REN_15d, REN_30d, REN_45d, REN_60d, REN_75d, REN_90d, REN_105d, and REN_120d, respectively.

We use a C++ code to manage implementation of MODFLOW-MT3DMS simulations. The code initially generates 5,000 sets of independent variables for each
scenario. The code generates the values of the seven inputs randomly with uniform distribution from their specified range shown in Table 3-1. The code also systematically applies the inputs of MODFLOW Model (i.e. constant head values in the eastern boundary, injection rate, ratio of extraction rate to injection rate, aquifer thickness, and hydraulic conductivity) and the inputs of MT3DMS model (i.e. porosity, longitudinal dispersivity, and aquifer thickness). Then, the C++ code runs MODFLOW and then MT3DMS codes and finally records the eight REN values (REN_15d, REN_30d,..., REN_120d) for each simulation.

3-3-4. Parallel processing

The computational demand for running 10,000 MODFLOW-MT3DMS simulations is enormous. For some sets of input variables, a single MODFLOW-MT3DMS simulation takes more than one hour (although for some others, run time is just a couple of minutes). To overcome this huge computational demand, we use parallel processing on a cluster of computing nodes, which can also be considered as a type of "cloud computing" (Hunt et al. 2010), to run multiple simulations in parallel.

Parallel processing is especially beneficial in groundwater studies because of the usual large computational demands for groundwater simulations (Ketabchi and Ataie-Ashtiani 2015). Several studies parallelized MODFLOW and MT3DMS codes to improve the computational efficiency of each individual simulation (Arnett and Greenwade 2000; Ji et al. 2014; Dong and Li 2009). Also, Dong et al. (2013) used a distributed parallel
processing for Monte Carlo type stochastic modeling in groundwater systems. Liu et al. (2013) and Hunt et al. (2010) presented two applications of cloud computing in groundwater studies.

In this study, we use Message Passing Interface (MPI) (Gropp et al. 2014, Neal et al. 2010), which is one of the most popular parallel programming techniques, to run MODFLOW-MT3DMS simulations in parallel. We convert the C++ code mentioned in the previous section from a serial code into a parallel code with MPI. To implement MPI, for example, on a single personal computer (PC), we virtually define a number of computing processors (independent of the number of the PC’s cores) to work simultaneously. One of the processors works as a “master” and the rest work as “slaves”. Initially, the master sends the inputs of a MODFLOW-MT3DMS simulation to each slave. The slaves run the MODFLOW-MT3DMS simulations and return the computed REN values to the master. Upon receiving REN values from a slave, the master sends the inputs of a new simulation to that slave. This process continues until finishing all simulations.

One can run an MPI code on a PC or on a cluster of computing nodes. Running the MPI code on a cluster of computing nodes can significantly decrease the total run time because it enables employing more processors as "slaves" which actually allows running more simulations in parallel. For this study, we use the cluster of computing nodes of the Center for High Performance Computing (CHPC) at the University of Utah. Provided that the computing nodes are available and idle, a member of CHPC can request even tens of computing nodes, each with multiple cores. This, in fact, allows
employing the number of machines that best suit the computational needs in each study. In order to exhibit the performance of parallel computing, we use "speedup" index (Gropp et al. 2014, page 32), which is the ratio of the serial execution time (Ts) to the parallel execution time (Tp).

\[
\text{Speedup} = \frac{T_s}{T_p}
\]  

(6)

3-3-5. ANN

Running all 10,000 MODFLOW-MT3DMS simulations and recording their corresponding REN results provides the input-output dataset needed for training ANN models. To train ANN models, we use "neuralnet" package (Fritsch and Günther, 2008) in R platform (R Core Team 2013). R is a free software which is an excellent environment for statistical computing and graphics. As mentioned before, as the structure of the model, we use three-layer feedforward ANN, which has one hidden layer. We use the nonlinear sigmoid activation function and the linear activation function for the hidden layer and the output layer, respectively. As the learning algorithm, we use the "resilient back-propagation with weight" method (Riedmiller, 1994) of the "neuralnet" package, which has shown superior performance than the traditional back-propagation technique.

Before using the data for ANN training, we normalize the values of each independent variable to be in the range of 0 and 1 using the maximum and minimum
values of that independent variable (Equation 7). Also instead of using REN values as a percentage value, we use them in the range of 0 to 1.

\[
\text{Normalized input value} = \frac{\text{Original value} - \text{Minimum value}}{\text{Maximum value} - \text{Minimum value}}
\]  

(7)

The number of nodes in the hidden layer is a design parameter. We determine the number of hidden nodes using the cross validation technique to prevent overfitting. We apply cross validation only on Scenario 1 data and consider its result as the optimal number of hidden nodes for ANN of Scenario 2, as well. To do cross validation, we use "repeated training-testing splits" or Monte-Carlo cross validation (Kuhn and Johnson 2013, page 71). First, we consider a set of values as the candidates for the number of hidden nodes. For each candidate model (with an assumed number of hidden nodes), we randomly split the original dataset (with 5,000 data) into training and testing subsets. We use 80% of the data (i.e. 4,000 data) for training and 20% of the data (i.e. 1,000 data) for testing. We train the candidate models with the training subset and then use the trained model to predict the outputs of the testing subset. Comparing the predicted outputs and observed outputs in the testing subset presents the performance of the trained model. We repeat this process 20 times for each candidate model and compute the performances average for each candidate model. If average performance of a candidate model becomes lower than performance of the models with less hidden nodes, this shows the onset of overfitting.
In order to measure the performance of models on testing subsets, we use root mean square error (RMSE), as shown in Equation 8. RMSE has the same unit of the dependent variable (herein REN) and implies how far, on average, the residuals (i.e. the difference between observed REN and predicted REN) are from zero. For illustration purposes, we also report the coefficient of determination ($R^2$), as shown in Equation 9.

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum (\text{REN}_O - \text{REN}_P)^2} \quad (8)$$

$$R^2 = 1 - \frac{\sum (\text{REN}_O - \text{REN}_P)^2}{\sum (\text{REN}_O - \overline{\text{REN}}_O)^2} \quad (9)$$

In Equations 8 and 9, N is the number of data in the testing subset, $\text{REN}_O$ are the observed values for REN, $\text{REN}_P$ are the predicted values for REN, and $\overline{\text{REN}}_O$ is the mean of observed values for REN. After finding the optimal number of hidden nodes using cross validation, we develop the final ANN models by training them using all 5,000 data.

### 3-4. Results

#### 3-4-1. MPI analysis

Before presenting the results related to ANN models development, we show the performance of MPI code employed for running MODFLOW-MT3DMS simulation in parallel. We conduct the performance analysis on a sample of 24 MODFLOW-MT3DMS simulations. The simulations are replicates (all of them have the same input values) because using different input values will result in different simulation run times, which
complicates the performance analysis. First, we investigate the efficiency of the MPI code on a personal computer (PC) with 8 cores. On the employed PC, a serial code needed 63.5 minutes to simulate those 24 simulations. Then, we run those 24 simulations in parallel using the MPI code by employing 2, 4, 6, 8, 12 and 24 processors as "slaves" and one processor as "master". Figure 3-3 shows the speedup (Equation 6) gained by employing MPI code on the PC. This figure shows that the maximum achievable speedup is 4.4 (i.e. it needs 14.4 minutes to run) using 8 slave processors. This means, using MPI code on the employed PC can reduce simulation times only by 4.4. Employing 12 or 24 slave processors even slightly reduces speedup. This is due to limitation in the number of processing cores and also memory in a single PC.

To show the performance of MPI code on a cluster of computing nodes, we first ran the 24 simulations in serial on one of the CHPC computing nodes and it took 69.1 minutes. Then, we used the MPI code to run those 24 simulations in parallel by employing 2, 4, 6, 8, 12 and 24 slave processors and one master processor using two CHPC computing nodes each with 12 cores. Figure 3-3 also shows the speedup gained by employing MPI code in CHPC. As shown, speedup continuously increases as the number of slave processors increases. For the tested example, speedup reaches 16.9 using 24 slave processors.

Obviously, the speed up of 4.41 achievable from a single PC is insufficient for the large number of simulations needed for this study. Therefore, practicality dictated that we run our MODFLOW-MT3DMS simulations using CHPC computing nodes. In one
access to CHPC resources, we employed 20 computing nodes each with 8 cores (in total 160 cores) to run 5,000 simulations of Scenario 1, and it took 7 hours and 43 minutes. In a separate access to CHPC resources, we were able to employ 20 computing nodes each with 12 cores (in total 240 cores) to run 5,000 simulations of Scenario 2, and it took 6 hours and 49 minutes. Note that for the same input values, one simulation of Scenario 2 takes longer than one simulation in Scenario 1 because Scenario 2 models have more stress periods. Based on the results obtained from Figure 3-3, we believe that we achieved speedup of about 80 for Scenario 1 simulations (when we used 160 processing cores) and speedup of more than 100 for Scenario 2 simulations (when we used 240 processing cores). This is a reasonable estimate for this study considering the
"embarrassingly parallel" nature of simulations, which means the runs are completely independent of each other and there is no interaction between slaves.

3-4-2. Data analysis

In order to examine the relationships between REN and the seven independent variables, we perform a correlation analysis using 5,000 input-output datasets of each scenario. This analysis reveals the relative importance of independent variables, and identifies the significant independent variables for use in the ANN models. Here, we use REN_90d as the representative value of REN. Table 3-2 shows the Pearson correlation coefficients for both Scenarios 1 and 2. Gradient, hydraulic conductivity, and aquifer thickness show a considerable negative correlation. This indicates that a larger value of these variables gives less REN. On the other hand, injection rate, ratio of extraction to injection rate, and porosity show a positive correlation.

In both scenarios, the strongest correlation is for gradient and hydraulic conductivity, therefore, these two are the most important variables on REN. The importance of gradient even increases by allowing one year storage of the injected water (Scenario 2). The weakest correlation is for longitudinal dispersivity especially for Scenario 2. Because the correlation coefficient of longitudinal dispersivity is negligible for Scenario 2 (i.e. equal to 0.01), we consider that as an insignificant independent variable and, therefore, we do not use it for making the ANN model for Scenario 2. However, we use longitudinal dispersivity as an input to make ANN for Scenario 1. Note
that because the inputs are randomly created values, there is no correlation between them, and the correlation coefficients are less than 0.02 for any pair of independent variables. In summary, we use all seven independent variables in Table 3-1 as inputs to develop the ANN model for Scenario 1, but we exclude longitudinal dispersivity for making Scenario 2 ANN.

Table 3-2. Correlation coefficients between REN_90d and independent variables

<table>
<thead>
<tr>
<th>Independent variables</th>
<th>Scenario 1</th>
<th>Scenario 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gradient</td>
<td>-0.65</td>
<td>-0.68</td>
</tr>
<tr>
<td>Hyd. Conductivity</td>
<td>-0.42</td>
<td>-0.4</td>
</tr>
<tr>
<td>Injection Rate</td>
<td>0.28</td>
<td>0.21</td>
</tr>
<tr>
<td>Ratio of Ext/Inj rate</td>
<td>0.24</td>
<td>0.16</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.18</td>
<td>0.16</td>
</tr>
<tr>
<td>Long. Dispersivity</td>
<td>-0.08</td>
<td>0.01</td>
</tr>
<tr>
<td>Aquifer thickness</td>
<td>-0.28</td>
<td>-0.27</td>
</tr>
</tbody>
</table>

3-4-3. ANN for Scenario 1

The ANN for Scenario 1 has seven nodes in the input layer and eight nodes in the output layer. The inputs are all seven independent variables shown in Table 3-1 and the outputs are eight values of REN_15d to REN_120d. To determine the optimal number of hidden nodes, we use cross validation by considering 3, 5, 8, 10, 15, 20, 25, 30, 35, 40, and 50 as the candidate numbers for hidden nodes. Figure 3-4 shows the results of cross validation.

Figure 3-4 shows the mean of RMSE and \( R^2 \) for 20 random resamplings used for each candidate model. The figure also shows 95% confidence interval for RMSE mean values
Figure 3-4. Cross validation profile to find the optimal number of hidden nodes of each candidate model. The numerically optimal value for the number of hidden nodes is 30 because it provides the least RMSE (and highest $R^2$). For the models with hidden node numbers more than 30, RMSE starts to increase or fluctuate, which is a sign of overfitting. Therefore, we consider 30 as the final result of cross validation. To have a more parsimonious ANN model, one could consider values 15-25 as the number of hidden nodes, since RMSE and $R^2$ do not improve significantly after these numbers.
Nevertheless, we choose 30 as the optimal number of hidden nodes for ANN models in this study.

Figure 3-5 shows the performance of the ANN with 30 hidden nodes on a testing subset (with 1,000 data shown with blue squares) after being trained with the associated training subset. In fact, Figure 3-5 shows the power of the developed ANN model for use as a predictive model.

![Figure 3-5](image)

Figure 3-5. Performance of Scenario 1 ANN on a testing subset (the red lines represent a 45 degree line showing the ideal prediction)
Figure 3-6 shows the residual plots for one of the REN values (REN_90d) for the same training-testing dataset used for Figure 3-5. As we see, the majority of residuals are within ±5% and residuals are randomly scattered about zero.

After confirming the predictability of the ANN model (with 30 hidden nodes) using training-testing subsets, we develop the final ANN model by training an ANN (with 30 hidden nodes) using all 5,000 data in Scenario 1.
3-4-4. ANN for scenario 2

The ANN for Scenario 2 has six nodes in the input layer and eight nodes in the output layer. The inputs are the independent variables shown in Table 3-1 except longitudinal dispersivity, which insignificantly affects REN for Scenario 2. The outputs are eight values of \( \text{REN}_{15d} \) to \( \text{REN}_{120d} \).

For consistency, we use the same number of hidden nodes determined for Scenario 1 ANN (equal to 30) for the ANN model of Scenario 2. Figure 3-7 shows the prediction ability of the Scenario 2 ANN model on a testing subset. Eventually, to develop the final ANN model for Scenario 2, we train an ANN with 30 hidden nodes using all 5,000 data in Scenario 2. It is worthwhile to mention that while other activation functions, more advanced neural networks, or even other machine learning techniques (e.g. Support Vector Machines) might provide higher accuracy, this was considered unnecessary for this study— the accuracy presented in Figures 3-5 and 3-7 is sufficient to satisfy the objective of this study, which is to develop a surrogate simulator that can rapidly estimate REN. Therefore, other alternatives were not investigated in this study.

3-4-5. Sensitivity analysis using ANN models

After finding the optimal number of hidden nodes, we can use the ANN models to identify the relative importance of independent variables for REN estimation. To do so, we create a training-testing dataset for each scenario. First, we train a complete
model (i.e. with all significant variables) using the training subset and evaluate its performance on the test subset for one of the REN values (REN_90d). Then, we repeat this process by systematically excluding one of the significant variables from the ANN model. The changes in performance (RMSE) of ANN models in comparison with the performance of the complete model reveal the relative importance of each input variable. Tables 3-3 and 3-4 show the results of this analysis for Scenarios 1 and 2.
Table 3-3. Sensitivity analysis using ANN model for Scenario 1

<table>
<thead>
<tr>
<th>Input variables used in ANN</th>
<th>RMSE(%)</th>
<th>R2</th>
</tr>
</thead>
<tbody>
<tr>
<td>All 7 significant variables</td>
<td>2.92</td>
<td>0.9903</td>
</tr>
<tr>
<td>All 7 significant variables but dispersivity</td>
<td>4.89</td>
<td>0.9728</td>
</tr>
<tr>
<td>All 7 significant variables but porosity</td>
<td>7.7</td>
<td>0.9327</td>
</tr>
<tr>
<td>All 7 significant variables but Ext/Inj ratio</td>
<td>9.12</td>
<td>0.9056</td>
</tr>
<tr>
<td>All 7 significant variables but injection rate</td>
<td>10.16</td>
<td>0.8843</td>
</tr>
<tr>
<td>All 7 significant variables but aquifer thickness</td>
<td>10.65</td>
<td>0.8712</td>
</tr>
<tr>
<td>All 7 significant variables but hyd. conductivity</td>
<td>14.95</td>
<td>0.7461</td>
</tr>
<tr>
<td>All 7 significant variables but gradient</td>
<td>23.86</td>
<td>0.3768</td>
</tr>
</tbody>
</table>

Table 3-4. Sensitivity analysis using ANN model for Scenario 2

<table>
<thead>
<tr>
<th>Input variables used in ANN</th>
<th>RMSE (%)</th>
<th>R2</th>
</tr>
</thead>
<tbody>
<tr>
<td>All 6 significant variables plus dispersivity</td>
<td>3.27</td>
<td>0.9921</td>
</tr>
<tr>
<td>All 6 significant variables</td>
<td>3.15</td>
<td>0.9926</td>
</tr>
<tr>
<td>All 6 significant variables but porosity</td>
<td>9.31</td>
<td>0.93</td>
</tr>
<tr>
<td>All 6 significant variables but Ext/Inj ratio</td>
<td>8.71</td>
<td>0.94</td>
</tr>
<tr>
<td>All 6 significant variables but injection rate</td>
<td>11.16</td>
<td>0.90</td>
</tr>
<tr>
<td>All 6 significant variables but aquifer thickness</td>
<td>12.32</td>
<td>0.89</td>
</tr>
<tr>
<td>All 6 significant variables but hyd. conductivity</td>
<td>19.39</td>
<td>0.72</td>
</tr>
<tr>
<td>All 6 significant variables but gradient</td>
<td>30</td>
<td>0.32</td>
</tr>
</tbody>
</table>

The results in Tables 3-3 and 3-4 are comparable with correlation analysis results in Table 3-2. Again, gradient and hydraulic conductivity show the highest importance—removing them from ANN models provides poor performance with high RMSE. It is interesting that inclusion of dispersivity within the ANN model of Scenario 2 causes an increase of RMSE. This exhibits that adding an insignificant variable to the ANN model
not only increases the complexity of the model, but can also damage the model performance.

3-4-6. Application of ANN models

The developed ANNs can be employed as a reconnaissance tool for immediate REN estimation for candidate hydrogeological or operational settings without the need to prepare and run MODFLOW-MT3DMS simulations. This is important knowing that a single MODFLOW-MT3DMS simulation can take more than one hour. Their fast estimation ability encourages ANNs inclusion within decision support systems (DSS) (Jakeman et al., 2011). A DSS should respond to "what if" questions rapidly (Anderson et. al., 2015, page 526). Using MODFLOW-MT3DMS models in DSS systems is not as attractive because of their usual long runtimes.

The ANNs also allow rapidly conducting sensitivity analysis of different independent variables on REN. In this section, we present the capability of the ANN models to conduct sensitivity analysis. For one year storage of injected water (i.e. Scenario 2) and assuming the ASR well is open only in one confined layer, we first evaluate the sensitivity of REN to the values of background gradient for the following conditions (which are close to the conditions of some JVWCD ASR wells):

- Aquifer thickness=61m
- Hydraulic conductivity=39.5m/d
- Porosity= 0.3
- Injection rate = 5,000 m$^3$/day
- Extraction rate = 10,000 m$^3$/day (Ratio of extraction to injection rate = 2)

Longitudinal dispersivity is not significant in Scenario 2, and therefore, the results are insensitive to changes in dispersivity. Figure 3-8 shows the changes in REN$_{90d}$ for 50 gradient values selected in its specified range (i.e. 0 to 0.004). This figure helps identifying the optimal locations for a proposed ASR well. For example, assuming other factors remain unchanged, installing the ASR well in a region with background gradient less than 0.0007 can provide REN$_{90d}$ of 100%. For gradient values more than 0.0007, REN$_{90d}$ can reduce significantly. Figure 3-8 demonstrates that the developed ANN models have captured the nonlinear relation between REN and independent variables. This allows better understanding of the changes in REN for each range of independent variables.

Assuming we have to install the well in a location with background gradient of 0.0015, the achievable REN$_{90d}$ is 63% (Figure 3-8). In order to improve REN, the ANN models allow investigating a change in operational factors of injection and extraction rates. Figure 3-9 shows the mutual impacts of injection rate and extraction rate on REN$_{90d}$ for this well. The figure has been obtained from a number of ANN simulations by changing the values of injection rates and ratio of extraction to injection rates (E/I) in their specified range while keeping other independent variables constant. This figure shows that an injection rate more than 7000 m$^3$/d and an E/I more than 2.5
Figure 3-8. REN_90d sensitivity to the values of background gradient for the assumed ASR well.

Figure 3-9. Mutual impact of injection rate and extraction rate on REN_90d for an ASR well located in a region with hydraulic conductivity of 39.5 m/d, gradient of 0.0015, aquifer thickness of 61m, and porosity of 0.3.
(i.e. extraction rate more than 17,500 m$^3$/d) is needed to achieve a REN_90d more than 90\% for the ASR well after one year storage of injected water.

It is worthwhile to mention that although we developed the ANN models for fully penetrating wells, they can also be used for REN estimation in partially penetrating wells, because the effect of partial penetration insignificantly affects REN. That means for a continuous screen interval, as long as the well is open in strata with the same horizontal hydraulic conductivity, we can approximate the achievable REN by entering the length of screen interval in the developed ANN models regardless of the total thickness of the aquifer.

Furthermore, although we developed the ANN models for one-layer systems, they can also be valid to approximate REN for ASR wells screened in multiple layers (with different horizontal hydraulic conductivity), assuming minimal vertical flow occurs between adjacent layers (e.g. in the presence of low values of vertical hydraulic conductivity) or if confining units exists between aquifer layers. Because each layer gets a proportion of total injected water based on its transmissivity ($T_i$), REN for each individual layer ($\text{REN}_i$) can be computed using ANN models and then the REN for the ASR well can be calculated by using Equation 10.

$$\text{REN}_{\text{well}} = \frac{\sum (\text{REN}_i \times T_i)}{\sum T_i}$$

(10)
3-4-7. Software development

The software developed here consists of the ANN models implemented in a stand-alone executable and a graphical user interface (GUI) to facilitate using the executable. By developing the final ANN models for Scenarios 1 and 2, we obtained a set of optimized weights as shown in Figure 3-1. We use these weights in equations similar to Equations 4 and 5 within the executable. The executable can compute REN for new input values within the range shown in Table 3-1.

The GUI and the ANN executable allow analyzing the sensitivity of REN to changes in one (as shown in Figure 3-8) or two independent variables (as shown in Figure 3-9), assuming other independent variables remain constant. Figure 3-10 shows a screenshot of the software as used to develop Figure 3-9. The GUI also has the capability of comparing the results of ANN models with the results of actual transport modeling (by invoking MODFLOW-MT3DMS models developed for Figure 3-2) for desired strategies. These strategies are usually the optimal strategies obtained during sensitivity analysis by ANN models.

3-4-8. Software availability

A free version of the developed GUI is available from peralta-web.bluezone.usu.edu.
3-5. Conclusions

We used REN as a performance criterion for ASR systems in freshwater aquifers. REN is the proportion of the injected water that the same ASR well can recover. We developed two ANN models to compute REN for two scenarios for storage of injected water. We obtained the input-output dataset needed for training ANNs from a series of MODFLOW-MT3DMS simulations.

Figure 3-10. A screenshot of the GUI developed for this study

We performed correlation analysis to select the significant variables for use in ANN models. Also, we conducted a sensitivity analysis using the developed ANN models
to reaffirm the relative importance of different independent variables within the ANN. Both analyses show that gradient and hydraulic conductivity have the highest impact on REN, and dispersivity has little impact, especially for Scenario 2 of storage duration (allowing 1 year of storage). The latter is fortunate since dispersivity is one of the hardest parameters to quantify in groundwater studies.

Using parallel processing is indispensable in this study because of the large number of MODFLOW-MT3DMS simulations needed for training the ANN models. For example, for simulations of Scenario 2, the prepared MPI code employed 240 processors from 20 nodes on a cluster of computing nodes. This provided 239 "slave" processors to run 239 simulations in parallel. We believe the speedup of this parallel run is more than 100, meaning the MPI code reduced run time of simulations in this scenario at least 100 times.

The developed software can be employed as a reconnaissance tool for immediate REN estimation for multiple numbers of hydrogeological or operational settings without the need to prepare and run multiple MODFLOW-MT3DMS simulations. Also, the developed software allows conducting sensitivity analysis of different independent variables on REN. For example, graphs such as Figure 3-9 can be developed for any ASR well (with parameters within Table 3-1 ranges) to investigate the effects of operational factors (i.e. injection and extraction rates) on achievable REN. Therefore, the software allows identifying superior hydrogeological or operational settings instantly.
References


McDonald, M.G. and Harbaugh, A.W., 1988. A modular three-dimensional finite-difference ground-water flow model.


CHAPTER 4
TRANSPORT MODELING AND MULTIVARIATE ADAPTIVE REGRESSION SPLINES FOR
EVALUATING PERFORMANCE OF ASR SYSTEMS IN FRESHWATER AQUIFERS

Abstract

We present a procedure using solute transport and statistical models to evaluate the performance of aquifer storage and recovery (ASR) systems designed to earn additional water rights in freshwater aquifers. The recovery effectiveness (REN) index quantifies the performance of these ASR systems. REN is the proportion of the injected water that the same ASR well can recapture during subsequent extraction periods. To estimate individual RENs, the presented procedure uses finely discretized groundwater flow and contaminant transport modeling. Then, the procedure uses multivariate adaptive regression splines (MARS) analysis to identify the significant variables affecting REN, and to identify the most recovery-effective wells. Achieving REN values close to 100% is the desire of the studied 14-well ASR system operator. This recovery is feasible for most of the ASR wells by extracting three times the injectate volume during the same year as injection. Most of the wells would achieve RENs below 75% if extracting merely the same volume as they injected. In other words, recovering almost all the same water molecules that are injected requires having a pre-existing water right to extract groundwater annually. MARS shows that REN most significantly correlates with groundwater flow velocity, or hydraulic conductivity and hydraulic gradient. MARS results also demonstrate that maximizing REN requires utilizing the wells located in
areas with background Darcian groundwater velocities less than 0.03 m/d. The study also highlights the superiority of MARS over regular multiple linear regressions to identify the wells that can provide the maximum REN. This is the first reported application of MARS for evaluating performance of an ASR system in fresh water aquifers.

4-1- Introduction

Aquifer storage and recovery (ASR) can help with balancing water supply and demand. ASR involves artificially recharging an aquifer through well(s) using surplus waters, for recovery during high-demand periods. The ASR practice can be cost-effective, while avoiding the evaporative and environmental concerns of surface reservoir use (Pyne 1995).

ASR wells exist in both saline aquifers (Ward et al. 2009) and freshwater aquifers. The criteria to quantify the performance of ASR systems in saline aquifers and freshwater aquifers differ. Here, we address an ASR system in a freshwater aquifer whose performance is defined as the amount of the injected water that the same ASR well can recapture. Forghani and Peralta (2017) introduced recovery effectiveness (REN) as the performance criterion of this type of ASR system (Equation 1).

\[ \text{REN} = \frac{V_{E_{\text{Inj}}}}{V_{I}} \]  

(1)

\( V_{E_{\text{Inj}}} \) is the volume of injectate existing within the volume of extracted water, and \( V_{I} \) is the volume of injected water.
The Jordan Valley Water Conservancy District (JVWCD) began operating part of the studied 14-well ASR system in a freshwater aquifer in Salt Lake County, Utah, in the year 2000 (Figure 4-1). The JVWCD developed this ASR system as a means of receiving additional water rights to supplement their pre-existing groundwater rights. The JVWCD desires to receive additional water rights equaling 100% of the injectate volume. However, the Utah Division of Water Rights (UDWR), which determines water rights for the region, assigns the additional water rights based upon the amount of the injected water that the same well can recover. Therefore, REN supports JVWCD-UDWR negotiations concerning allocation of additional water rights to the JVWCD.

The JVWCD performed extensive testing using natural tracers to track the injected water and estimate REN. However, the results could only show general trends, such as the gradual reduction of injectate recovery with time (SLCWCD 1996). Field techniques were unable to reasonably and accurately estimate REN. This caused the need for a defensible modeling-based procedure to estimate REN.

The study presents a practical procedure to evaluate REN for ASR systems in freshwater aquifers using transport modeling and statistical analysis. The procedure addresses two objectives: 1) estimating overall REN using transport modeling, and 2) statistically identifying significant hydrogeologic parameters affecting REN, and identifying the most recovery-effective wells. In order to address objective 1, we quantify REN for each of 14 JVWCD ASR wells using MODFLOW (McDonald and Harbaugh 1988) and MT3DMS (Zheng and Wang 1999) simulations. We address
objective 2 by using the results of MODFLOW-MT3DMS simulations in a piecewise linear regression model called multivariate adaptive regression splines (MARS) (Friedman 1991). This study is the first reported application of MARS for evaluating REN in an ASR system in freshwater aquifers.

Figure 4-1. The JVWCD ASR area

4-2- Multivariate adaptive regression splines (MARS)

Multivariate adaptive regression splines (MARS) is a non-parametric regression technique (i.e. the shape of the relationships between predictors and response is not
predetermined) that provides results in a form similar to multiple linear regression (MLR), while revealing essential nonlinearities (Friedman 1991). Unlike MLR, which provides one slope for each significant variable, MARS can present different slopes (i.e. piecewise linear relations) for different ranges of a significant variable space (Emamgolizadeh et al 2015; Kisi and Parmar 2016). Therefore, in comparison with MLR, MARS provides more information for interpreting how each significant variable affects the dependent variable (i.e. REN in this study). Figure 4-2 presents a typical result of MARS for independent variable X (Equation 2).

![Figure 4-2. A typical result of MARS model](image)

In Figure 4-2, C is a cut-point for variable X. Assuming variable X has only this cut-point, two pairs of “hinge” functions can be potentially created for variable X:

\[
Y = \max(0, x - C) = \begin{cases} 
0 & \text{if } x < C \\
(x - C) & \text{if } x > C
\end{cases}
\] (2)

\[
Y = \max(0, C - x) = \begin{cases} 
C - x & \text{if } x < C \\
0 & \text{if } x > C
\end{cases}
\] (3)
MARS automatically finds the value C among variable X data points such that the selected value provides the best model fit (e.g., the least RMSE for model residuals). Instead of merely using the original independent variables (i.e., here X), MARS adds hinge functions into a simple linear regression. If including the hinge functions improves the model fit, MARS retains them in the model and estimates their slopes. MARS repeats this process for all independent variables, developing hinge functions (and their corresponding slopes) that can improve (even slightly) the model fit.

After providing a model with all helpful hinge functions, MARS performs a “pruning” process in which it removes the hinge functions that do not contribute significantly to the model fit. This provides a more parsimonious model with less probability of suffering from overfitting (Kuhn and Johnson 2013, Chapter 7).

Above text describes the process for an additive MARS where there is no interaction between independent variables. This is called a MARS with degree one. MARS with degree higher than one can consider interactions between independent variables. To do so, MARS examines products of hinge functions of different independent variables.

4-3- Methodology

The following subsections detail the development of a transport model to quantify REN for ASR wells. We model the operations of JVWCD ASR wells using a 5-year monthly model. For accurate transport modeling, we refine the model in the area of ASR
wells. After preparing a refined flow model, we utilize transport modeling. The solute transport model simulates the movement of water injected in year 1 during the next five years of ASR operation and calculates REN for each well.

4-3-1- Previous modeling studies

The most reliable groundwater modeling studies available in the region are a series of studies by the USGS (Lambert 1995a, Lambert 1995b, Stolp 2007). The USGS developed a MODFLOW model with yearly stress periods to simulate groundwater flow in Salt Lake Valley (Lambert 1995a). The simulated heads represent heads in months January-February. The model was calibrated to steady state conditions of year 1968 and to transient state of years 1969 to 1992. The model has 94 rows and 62 columns, with each cell 563.3m on a side. Vertically, the model divides the groundwater system into seven layers. Layers 1 and 2 represent a shallow unconfined aquifer and an underlying semi-confining unit in the center of the valley. Layers 3 to 7 constitute the principal aquifer, where all ASR wells are screened. We used the calibrated USGS MODFLOW model (Lambert 1995a) as the basis when preparing a flow model for this study.

4-3-2- Evaluating the accuracy of the USGS model for the current time

Although the aquifer parameters calibrated by the USGS study have been used in several transport studies (Lambert 1995b, Lambert 1996, Stolp 2007, Jeffrey et al. 2014), before using them for this study, we evaluate their accuracy to simulate the
groundwater system under current hydrological stresses. To do so, we extend the USGS model with the updated yearly stresses representing hydrologic conditions from 1993 to 2014. Then we evaluate the accuracy of the 1993-2014 model by comparing its results with observed heads in observation wells.

4-3-3- Preparing a monthly flow model

After confirming the applicability of the USGS MODFLOW model for the current time, we simulate a monthly ASR operation scenario provided by JVWCD (written communication with JVWCD). The scenario has 60 monthly stress periods within five years. In order, the five years represent average, dry, dry, wet, and average hydrological conditions. The scenario also includes hydrologically varying estimates of the background stresses (e.g. non-ASR supply wells and recharges). Initial conditions are January 2009 heads resulting from simulations of the 1993-2014 model described in the previous section.

Background stresses for average years are the monthly average values of the stresses in years 2009-2014 based on the best estimate of monthly data in the region. Multiplying average year stresses by reasonable coefficients produces the stresses for dry and wet years. For instance, extraction from non-ASR supply wells in dry and wet years, respectively, equal 1.2 and 0.6 times average year extraction (written communication with JVWCD).
Regarding the ASR wells operational scenario, all five years employ unchanged injection and extraction rates. To represent the effect of different hydrological conditions, wet years and dry years have different injection and extraction durations than average years. Dry years (years 2 and 3) have no injection (written communication with JVWCD). Injection occurs from April through June and extraction occurs from July through September. For years with injection (average or wet years), the ASR well pumping rates and durations are such that a significant extraction—at least three times the injection volume—occurs in the same year as injection (usually within 3-4 months after injection).

We use the MODFLOW MNW2 package (Konikow et al. 2009) to model ASR wells operation, whereas the other background pumping wells are modeled by the original WEL package. Most JVWCD ASR wells are screened in multiple model layers in the principal aquifer. The MNW2 package improves the accuracy of simulating multilayer wells (Neville and Tonkin 2004).

4-3-4. Preparing a refined flow model

The USGS flow model has cell sizes of 563.3m by 563.3m. Transport modeling using this model cannot provide a reasonable REN estimation. Forghani and Peralta (2017) show the importance of employing horizontally refined models for an accurate REN estimation. They present a procedure to prepare sufficiently refined models using telescopic mesh refinement (TMR) (Leake and Claar 1999) and local grid refinement.
(LGR) (Mehl and Hill 2013) techniques to quantify REN for one ASR well. However, these methods are tedious to implement for modeling a group of ASR wells located in a relatively large area within the original model domain. TMR and LGR techniques work best for modeling a limited portion of an original model.

Here, we use the variable mesh refinement technique using ModelMuse (Winston 2009) to prepare a horizontally refined model. No vertical refinement is implemented because preliminary simulations showed that vertical refinement does not change the accuracy of REN estimation. We make the cell sizes in the area of ASR wells as small as 10m by 10m. We refine the rest of the model such that the ratio of cell sizes between any two neighboring cells is not larger than 1.5. The employed refinement technique also refines the MODFLOW river cells adjacent to ASR wells (Figure 4-1). Reckless refinement of river cells can cause unrealistic simulated groundwater heads. After grid refinement, we use a GIS map of the Jordan River to accurately determine the location and conductance values of river cells.

4-3-5. Transport modeling

After preparing the refined flow model, we utilize transport modeling with MT3DMS code. To distinguish injected water from native groundwater (because both are freshwater with similar qualities), we assume injected water has an imaginary non-reactive contaminant. We model the injected water with an arbitrary concentration of 100 ppm while assuming zero concentration for native groundwater. We track the
"contamination" injected in year 1 during the 5-year simulated ASR operation. REN (Equation 1) equals extracted "contamination" divided by the year 1 injected "contamination".

Because both injected water and native groundwater are freshwaters of similar quality, using the MT3DMS reaction package is dispensable. We use the total variation diminishing (TVD) technique as the solution method in MT3DMS to minimize numerical dispersion (Zheng and Bennett 2002). To reduce the run time of the transport model, in MT3DMS model, we make the cells distant from the ASR field inactive. Emulating another USGS study (Lambert 1995b), we use an effective porosity of 0.4 for layers 1 and 2, and an effective porosity of 0.3 for principal aquifer (layers 3 to 7).

Both advection and dispersion packages of MT3DMS model are necessary for an accurate REN estimation (Lowry and Anderson 2006, Forghani and Peralta 2017). A judicious choice of dispersivity values is one of the most challenging parts of transport modeling (Konikow 2011). In practice, dispersivity values are usually obtained during calibration. Also, many studies have shown that longitudinal dispersivity values generally depend on the scale of observations (Gelhar 1992, Schulze-Makuch 2005, Xu and Eckstein 1995). Lacking reliable observation data for calibration, we estimate longitudinal dispersivity ($\alpha_L$) using Equation 4 (Xu and Eckstein 1995). The scale equals the largest expected length of injectate plume ($L_P$).

$$\alpha_L = 0.83\log_{10}(L_P)^{2.414}$$
We categorize the ASR wells into two groups: 1) ASR wells with long plume length (mostly for the wells located in regions with high gradient and high hydraulic conductivity), and 2) ASR wells with short plume length. Based on the longest expected injectate plume ($L_P$) in each group, the dispersivity values in groups 1 and 2 are estimated 7m and 4.5m, respectively. Horizontal and vertical transverse dispersivities are one and two orders of magnitude smaller than longitudinal dispersivity, respectively.

4-4. Results and discussion

4-4-1. Accuracy of the USGS model for the current time

As mentioned, before using the USGS flow model for this study, we evaluate the accuracy of the model to predict the observed heads at the current time. Figure 4-3 compares the observed heads (in month February) and the model-simulated heads in year 2014 for 35 observation wells in the region. The 95% confidence interval (CI) lines show the joint confidence interval for the regression line at the values of X axis (observed heads) by the Scheffe method (Brown and Hollander 1977, p. 271-274). The Y axis represents model-simulated heads. This figure shows that only 5 out of 35 observation wells lie outside the 95% confidence interval.

Also, residuals of the USGS 1969-1992 model and the model developed here for years 1993-2014 are similar. Figure 4-4 compares the residual changes between the two models for one of the observation wells. In general, the accuracy obtained for the 1993-2014 model is comparable with the accuracy of the USGS calibrated model. Therefore,
we use the aquifer parameters from the USGS model to simulate the region’s groundwater for the current time.

4-4-2. Flow model reliability

Preparing a refined model with a good mass balance error (less than 1%) is often difficult when using variable grid refinement technique (Mehl and Hill 2006). This difficulty arises mostly from the existence of cells with different sizes in a same model. In the refined model, we have cell sizes as large as 563m and as small as 10m. Herein, reducing the mass balance error to about 1% involves decreasing the head change criterion for convergence (HCLOSE term in MODFLOW) and also increasing the number
of solver iterations (McDonald and Harbaugh 1988). These increase the runtime of this 60-period flow model.

Figure 4-4. Similarity in residual changes between the two models for one of the observation wells

Nevertheless, the results of the refined flow model are reasonable. Figure 4-5 shows monthly averaged simulated aquifer discharge to the Jordan River in simulated years 1-5. This figure presents the model’s responsiveness to different hydrological conditions in this study.
Figure 4-5. Monthly averaged simulated aquifer discharge to the Jordan River

Also, the values of head-dependent boundaries in the mass balance table of the refined model are reasonably comparable to the values from the regional model before refinement. This consistency for river cells was achieved after updating the location and the conductance values of the river cells in the refined model. For example, for the first year, Figure 4-6 presents the improvement in the simulated aquifer discharge into the Jordan River achieved by revising river package data.

4-4-3. Transport model results

After confirming the reliability of the refined flow model to simulate the hydraulic gradients of ASR wells during ASR operations, we conduct transport modeling to estimate REN for the JVWCD ASR wells. Figure 4-7 presents the results of the
transport simulation. This figure compares $\text{REN}_{\text{Final}}$, the final achievable REN after five years of ASR operation, with $\text{REN}_{\text{RATIO1}}$, $\text{REN}_{\text{RATIO2}}$, and $\text{REN}_{\text{RATIO3}}$. $\text{REN}_{\text{RATIO1}}$, $\text{REN}_{\text{RATIO2}}$, and $\text{REN}_{\text{RATIO3}}$ denote the achieved REN by extracting one, two, and three times of injectate volume, respectively.

As mentioned before, due to pre-existing groundwater pumping rights, the pumping scenario allows the ASR wells to extract at least three times the injectate volume during the same year as injection. This is the key to provide high REN values in this system. Except for three wells, SLC3, SLC22, and SLC28, all wells have REN of almost 100%. The background gradient at wells SLC3, SLC22, and SLC28 (located in the eastern margin of the valley) is greater than the other wells.
The weighted average REN (i.e. overall REN) for the entire system is about 98% after 5 years of simulated ASR operation. Note that model results show that no water injected by one well is captured by other wells. Therefore, all reported REN values in Figure 4-7 represent the amount of the injectate water into a well that is captured by the same well.

Figure 4-7 also demonstrates two important findings. First, extracting the same amount of injectate volume will achieve REN not more than 75% for most wells (see REN_{ratio1} values). This highlights the importance of having pre-existing water rights to achieve a very high REN. Second, most of the final achievable REN occurs while extracting three times the injection volume (by achieving REN_{ratio3}), and further extraction cannot significantly increase REN. This is especially evident for three wells in
high-gradient regions. After extracting three times the injection volume, the injectate either has been captured by the well, or has departed the well’s capture zone. In Figure 4-7, the $R_{\text{EN\text{Ratio3}}}$ values average 2% less than $R_{\text{EN\text{Final}}}$ values. Therefore, $R_{\text{EN\text{Ratio3}}}$ can be a reasonable approximator of the final $R_{\text{EN}}$ in this system.

Although we assumed a hydrologic sequence of average, dry, dry, wet, and average, other sequences provide comparable results. This occurs because the ASR wells always extract at least three times the injected volume during the same year as injection, making their performance (i.e. $R_{\text{EN}}$) independent of a specific hydrologic condition.

Also, for injection volumes lower than the injection volume in this study (about three million cubic meters), the overall $R_{\text{EN}}$ would be higher than 98% estimated in this study. This occurs because this ASR system must operate annually in order to satisfy water demands. If less surplus water is available for injection, and therefore, less water (than we simulated in this study) is injected, the system will provide a higher ratio of extracted volume to injected volume, producing $R_{\text{ENs}}$ higher than the values shown in Figure 4-7.

4-4-4. Regression analysis

To identify the significant variables affecting $R_{\text{EN}}$, we apply the MARS regression technique on the results of transport modeling (i.e. Figure 4-7). MARS also provides
piecewise linear relations between significant variables and REN, and identifies the range for each significant variable that provides maximum RENs.

$\text{RENRATIO3}$ is the dependent variable in the analysis. This imposes commensurate extraction volumes for all wells. The analyzed independent variables are background gradient, hydraulic conductivity ($K$), total well screen length, and injection volume (Table 4-1). We estimate background gradient for each well using heads simulated by the refined flow model for the time just before injection. Equation 5 computes the wells’ hydraulic conductivity:

$$K_{x,\text{ave}} = \frac{\sum(k_{x,i} \times b_i)}{\sum b_i}$$

(5)

$k_{x,i}$ and $b_i$ are the horizontal hydraulic conductivity and aquifer thickness for layer $i$, respectively. The total screen length equals $\sum b_i$. For a properly constructed statistical model, MARS identifies significant variables and formulates a function to compute $\text{RENRATIO3}$.

Table 4-1. Independent and dependent variables used for statistical analyses

<table>
<thead>
<tr>
<th>Number of data (N)</th>
<th>Independent variables</th>
<th>Dependent variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>$K$, Gradient, Screen length, Injection volume</td>
<td>$\text{RENRATIO3}$</td>
</tr>
</tbody>
</table>
4-4-4-1. MARS results

MARS analysis identifies gradient and hydraulic conductivity (K) as significant variables. The resulting Equation 6 has an R-squared ($R^2$) of 0.96.

$$RENRATIO3 = 98 - 1224 \times \max(0, \text{Gradient} - 0.0018) - 0.17 \times \max(0, K-20) \quad (\text{Equation 6})$$

Equation 6 states that ASR wells with $k$ less than 20 m/d and gradient less than 0.0018 provide $RENRATIO3$ of 98%. Below those values, gradient and K terms do not reduce $RENRATIO3$, and extracting three times the injectate volume will achieve a 98% REN. $K$ values more than 20 m/d will reduce REN based on the relationship below:

$$0.17 \times (K-20)$$

Similarly, gradient values more than 0.0018 will reduce REN based on the relationship below:

$$1224 \times (\text{Gradient} - 0.0018)$$

Figure 4-8 shows the results graphically.

By also including the product of gradient and hydraulic conductivity (i.e. the background Darcian velocity), MARS produces Equation 7 (with $R^2$ of 0.97). Equation 7 states that velocity ($V$) is the only significant variable.

$$RENRATIO3 = 98 - 58 \times \max(0, V - 0.03) \quad (7)$$

Equation 7 implies that:

For $V<0.03$ m/d (applicable for eight ASR wells): $RENRATIO3=98 \quad (7a)$

For $V>0.03$ m/d (applicable for six ASR wells): $RENRATIO3=98-58\times(V-0.03) \quad (7b)$
Figure 4-8. Graphical demonstration of MARS results in Equation 6

Figure 4-9 illustrates the MARS model results of Equation 7. This figure also shows the observed data (from transport model) with blue squares. Note that the models in Equations 6 and 7 are from an additive MARS model (i.e. using degree one). Using MARS with degree two did not provide a more accurate model and was unnecessary in this study.

MARS cannot provide confidence intervals (Milborrow 2017). To obtain approximate confidence intervals for the intercept in Equation 7a, we use a simple linear regression for the data with $V<0.03\text{m/d}$ (eight data). The result is shown in Equation 8a, where the 95% confidence interval for the intercept is $(96.2, 99.2)$.

\[ \text{REN}=97.7\% \quad (8a) \]

Similarly, using a simple linear regression for the data with $V>0.03\text{m/d}$ (six
data) provides Equation 8b, where the 95% confidence interval for the velocity coefficient is (-74, -44).

\[ \text{REN}_{\text{RATIO3}} = 100 - 58.8 \times V \]  

(8b)

Figure 4-9. MARS model developed to explain the JVWCD ASR system

The MARS model (Equation 7 or Figure 4-9) explains the observed data of the JVWCD ASR system very well (i.e. R2=97%). However, caution is needed in use of this model for REN prediction at other locations. Using the average injection volume (210,000m³) and the average screen interval length (100m), supplementary transport simulations show that the MARS model reliably predicts REN for velocities up to 0.1m/d. This is consistent
with the limited number of data (i.e. three data) having velocity more than 0.1m/d in Figure 4-9. Also, note that although injection volume and screen interval length are insignificant variables for the JVWCD ASR system, they might be significant for other ASR systems.

4-4-4-2. Comparison of MARS and multiple linear regression

To compare with MARS results in Equation 6, and to identify the relative importance of significant variables, we also apply multiple linear regression (MLR) to the transport modeling results. Using K, gradient, screen length, and injection volume as independent variables, Table 4-2 shows the best model developed using MLR. The adjusted R-squared ($R^2$) value is 0.94.

Table 4-2. The best model developed using multiple linear regression

<table>
<thead>
<tr>
<th>Variables</th>
<th>Regression Coefficients</th>
<th>t value</th>
<th>P value</th>
<th>Standardized coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Intercept)</td>
<td>100</td>
<td>143</td>
<td>2.00E-16</td>
<td>NA</td>
</tr>
<tr>
<td>Gradient</td>
<td>-1145</td>
<td>-13.6</td>
<td>8.90E-08</td>
<td>-0.94</td>
</tr>
<tr>
<td>K (m/d)</td>
<td>-0.076</td>
<td>-2.34</td>
<td>0.0413</td>
<td>-0.16</td>
</tr>
</tbody>
</table>

Similar to MARS, MLR identifies gradient and K as significant variables (with P values less than 0.05, where P values demonstrate significance level of estimated coefficients). However, MLR, does not identify cut-points within significant variable spaces. For
example, MLR suggests applying a coefficient of -0.076 for the entire range of K values to compute its effect on REN. MARS Equation 6, however, showed that K negatively impacts REN only for K values exceeding 20m/d. Also note that for K exceeding 20m/d, MARS proposes a steeper slope than MLR. In contrast to MARS, MLR proposes an average slope for the entire range of significant variables instead of providing relevant information for different ranges of variable space.

Table 4-2 also shows the standardized coefficients which display the relative importance of significant variables. Standardized coefficients are the regression coefficients obtained by making a separate MLR model after normalizing the independent variables data. As shown in Table 4-2, gradient is almost six times more important than hydraulic conductivity, highlighting the crucial importance of background gradient on achievable REN.

4-5. Conclusion

We utilize flow and transport simulation to estimate REN for 14 wells in an ASR system in a freshwater aquifer. REN, the performance index of the studied ASR system, represents the proportion of the injected water that the same wells can recover. Preparing a reliable refined flow model involves evaluating the adequacy of a previously calibrated regional flow model for groundwater simulation at the current time. Estimating REN in this freshwater aquifer requires distinguishing the fresh injected
water from the fresh native groundwater. Thus, solute transport simulation employs imaginary contamination in the injected water.

Transport simulation results show that the studied ASR system can achieve 98% of the injected water within five years of ASR operation. Most of this recovery results from extracting three times the volume of injection during the same year as injection. Extracting more than three times of injectate volume does not significantly improve REN. Extracting merely the same amount as the injectate volume achieves RENs not more than 75% for most of the wells. This emphasizes the importance of having pre-existing water rights to achieve a satisfactory performance for this type of ASR systems.

MARS statistical analysis identifies background hydraulic gradient and hydraulic conductivity (or background Darcian velocity) as the most significant parameters affecting REN in the studied system. MARS finds threshold values within significant variables spaces and provides equations for estimating REN within each section of each significant variable space. For instance, MARS suggests that hydraulic conductivity (K) can negatively impact REN (with a specified coefficient) only for the wells with K more than 20m/d. MARS also shows that for a well located in an area with background Darcian velocity less than 0.03m/d, the maximum REN (i.e. 98%) is achievable after extracting three times the injectate volume.
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CHAPTER 5

USING GENERALIZED NEURAL NETWORKS FOR MIXED INTEGER MULTI-OBJECTIVE
OPTIMIZATION OF ASR SYSTEMS IN FRESHWATER AQUIFERS

Abstract

This paper presents an integrated simulation-optimization model to aid managing the performance of ASR systems in freshwater aquifers. The recovery effectiveness (REN) index quantifies the performance of the studied ASR system. The REN is the injectate proportion that is recoverable from the same well during subsequent extractions. The study addresses this ASR system when used for yearly storage of injected water. The proposed model couples the multi-objective genetic algorithm NSGA2 with a generalized surrogate simulator capable of estimating REN in partially penetrating wells screened in multiple strata. The surrogate simulator employs neural networks to circumvent the need for running computationally intensive transport simulations. Two decision variables of each well are injection rate and extraction duration which are modeled as real and discrete variables, respectively. Results of the optimization scenarios categorize the system's 14 ASR wells into three rankings based on their recovery effectiveness. The wells’ rankings allow the system’s managers to decide which ASR wells to operate in order to maximize the system’s REN. This is the first study that uses optimization models to maximize the overall REN in an ASR system while addressing partial penetrating wells screened in multiple strata.
**5-1- Introduction**

Aquifer storage and recovery (ASR) involves artificially recharging an aquifer through well(s) using surplus water for later recovery in high-demand months. The ASR can help with preventing the decline of groundwater levels and balancing water supply and demand. As a water management alternative, the use of the ASR wells is growing due to increasing concern about the environmental impacts of surface reservoir use (Pyne, 1995). Water managers can operate ASR wells in both saline aquifers (Ward et al., 2009; Barker et al., 2016) and freshwater aquifers (Forghani and Peralta, 2017c).

In this study, we employ simulation and optimization models to optimize the performance of an ASR system in a freshwater aquifer. The Jordan Valley Water Conservancy District (JVWCD) began operating this ASR system in Salt Lake County, Utah, in the year 2000 (Figure 5-1). By injecting the extra surface water into the aquifer in wet months, the JVWCD desires to receive additional water rights to supplement their pre-existing groundwater rights for use in dry months. However, the Utah Division of Water Rights (UDWR), which determines water rights for the region, determines the additional water rights based upon the proportion of the injected water that is recoverable from the same wells. Therefore, we use the recovery effectiveness (REN) index to quantify the performance of the JVWCD ASR system (Forghani and Peralta 2017a).

\[
REN = \frac{V_{E\text{Inj}}}{V_I}
\]  

(1)
where $V_{E_{\text{inj}}}$ is the volume of injectate existing within the volume of extracted water, and $V_I$ is the volume of injected water.

Figure 5-1. The JVWCD ASR project Area

Forghani and Peralta (2017c) investigated this ASR system and concluded that the system's overall REN is more than 95%, if the wells extract three times their
injection volume in the same year of injection (typically within 3-4 months after injection). This is feasible due to pre-existing groundwater pumping rights in this ASR system.

This paper addresses this ASR system for the conditions of storing the injectate in the aquifer for a year—injecting into aquifer in spring months of year 1 and extracting from the wells in dry months of year 2 (i.e. after 12 months of storage). The addressed objectives of the system are: 1) maximizing the system's overall REN at the end of year 2, 2) minimizing the system's total extraction volume, and 3) minimizing the pumping costs.

We use the multi-objective genetic algorithm NSGA2 (Deb et al., 2002) with mixed discrete-continuous decision variables to identify the wells' optimal injection rates in year 1 and extraction durations in year 2. As the REN simulator in the coupled simulation-optimization model, we use generalized artificial neural networks (ANNs) developed by Forghani and Peralta (2017b). To mitigate the computational burden, many groundwater studies have used surrogate simulators (e.g. regression equations or neural networks) to replace the flow or transport simulations (Aly and Peralta, 1999; He et al., 2008; Fayad et al., 2012; Peralta et al., 2014). However, most of the surrogates reported in the literature belong to a specific area and are applicable only for the studied region. By presenting the accuracy of the ANN models developed by Forghani and Peralta (2017b) to estimate REN in partially penetrating wells screened in multiple
strata, this paper also introduces these ANNs as a viable tool for estimating REN in many ASR systems worldwide.

The results of the optimization scenarios categorize the 14 JVWCD ASR wells into three rankings regarding their recovery effectiveness for a yearly storage of injected water. The study employs the wells’ rankings to suggest operational guidelines in order to maximize the overall REN in the studied ASR system.

5-2- Materials and Methodology

5-2-1. Generalized Neural Networks to Estimate REN

Forghani and Peralta (2017b) developed two generalized ANN models to rapidly estimate REN for two injectate storage conditions: 1) allowing minimal storage of injected water (i.e. extraction begins immediately after injection), and 2) allowing one year storage of injected water (i.e. extraction begins after storing the injected water in the aquifer for 12 months). Both ANNs assume injecting into the aquifer for two months, which is a reasonable injection duration for many ASR systems, including the JVWCD system.

Forghani and Peralta (2017b) implemented 10,000 transport simulations using MODFLOW (McDonald and Harbaugh, 1988) and MT3DMS (Zheng and Wang, 1999) to create the dataset needed for training and validating the ANNs. Dataset inputs include all factors that can significantly affect REN in freshwater aquifers. These seven factors are background hydraulic gradient (which is usually estimated from a calibrated regional
model), hydraulic conductivity, aquifer thickness, porosity, longitudinal dispersivity, injection rate, and extraction rate. Dataset outputs are computed RENs for each 15 days of extraction up to 120 days.

Before developing the ANNs, a correlation analysis showed that longitudinal dispersivity has little correlation with REN for yearly storage conditions. Therefore, among the aforementioned seven factors, longitudinal dispersivity was excluded for making the ANN model for the yearly storage condition. This is fortunate because estimating dispersivity is one of the most challenging parts of transport modeling (Konikow, 2011). The developed ANNs are useful to estimate REN in freshwater aquifers for any ASR system whose parameters are within the range of the parameters used to develop the ANNs. Forghani and Peralta (2017b) present more details about the ANN models and their accuracy.

Although the ANN models have been developed for fully penetrating ASR wells in one-layer systems, they can also be used for REN approximation in partially penetrating wells screened in multiple strata (with different horizontal hydraulic conductivities). During injection, each stratum receives a proportion of the total injected water based on its transmissivity ($T_i$). When there is a minimal vertical flow between adjacent layers (e.g. in the presence of low values of vertical hydraulic conductivity, or if confining units exist between aquifer layers), injected water in each stratum behaves independent of other strata, and REN of each layer ($\text{REN}_i$) can be computed using ANN models. Then, Equation 2 can approximate REN for the entire ASR well.
\[ R_{\text{EN,well}} = \frac{\sum (R_{\text{EN},i} \times T_{i})}{\sum T_{i}} \]  

(2)

In this study, we use ANN models with Equation 2 to estimate REN in ASR wells. For most of the JVWCD ASR wells, the vertical hydraulic conductivity is much less (less than 5%) than horizontal hydraulic conductivity.

5-2-2. A regional MODFLOW-MT3DMS model

In order to verify the accuracy of the ANN models for REN prediction in multi-layer wells, it is required to prepare a transport model using MODFLOW and MT3DMS. The regional MODFLOW model is also required to estimate the background hydraulic gradient (the gradient before starting an ASR operation), which is one of the ANNs inputs for each ASR well. In addition, the MODFLOW model can compute water levels inside wells during ASR operations.

We use a USGS calibrated MODFLOW model with yearly stress periods developed to simulate groundwater flow in Salt Lake Valley (Lambert, 1995). In order to simulate the 2-year ASR operation needed in this study, we convert two years of the USGS model into 24 monthly periods. Vertically, the model divides the groundwater system into seven layers. Layers 3 to 7 constitute the principal aquifer. All ASR wells are open in multiple model layers in the principal aquifer. To improve the accuracy of simulating multi-layer wells, and also to compute water levels inside the wells, we use the MODFLOW MNW2 package (Konikow et al., 2009; Neville and Tonkin, 2004) for
modeling the ASR wells. The MNW2 package considers the effects of partial penetration and aquifer loss (the effect of well radius) to accurately compute the water level in each well. The JVWCD wells have a 40 or 50cm casing diameter.

Horizontally, the USGS model has cell sizes of 563.3m by 563.3m. For an accurate REN estimation, we need to prepare a horizontally more refined model. To do that, we use the variably mesh refinement technique using ModelMuse (Winston, 2009). No vertical refinement is required because preliminary simulations showed that REN is insensitive to vertical refinement. We reduce the cell sizes in the area of ASR wells to 10m by 10m. The rest of the model is refined such that the ratio of cell sizes between any two neighboring cells is not larger than 1.5.

Because both injected water and native groundwater are freshwaters with similar qualities, to distinguish injected water from native groundwater, the developed MT3DMS model assumes an imaginary non-reactive contamination in the injected water. REN (Equation 1) is quantified as the extracted "contamination" from the well divided by the injected "contamination". Lacking reliable observation data for calibration, we estimate longitudinal dispersivity by applying the ASR scale within the Xu and Eckstein (1995) formula. Here, the scale for each ASR well equals the injectate plume length during an ASR operation. In order to minimize numerical dispersion (Zheng and Bennett, 2002), we use the total variation diminishing (TVD) technique as the solution method in MT3DMS.
5-2-3. Multi-objective optimization

In a multi-objective optimization problem, there exists a set of solutions known as Pareto or nondominated solutions. Solution A dominates solution B—A is nondominated compared to B if: 1) A is not worse than B in all objectives, and 2) A is better than B in at least one objective (Deb, 2001; Sreekanth and Datta, 2010).

Traditional multi-objective optimization techniques, such as weighting and E-constraints methods, convert a multi-objective problem into a single-objective problem (Major, 1977; Peralta and Kalwij, 2012; Peralta et al., 2014). The weighting method applies user-specified weights to the objectives to define a new hybrid objective. The E-constraint method keeps only one of the objectives and converts the other objectives into constraints (Datta and Peralta, 1986; McPhee and Yeh, 2004). Afterwards, the classic or heuristic methods are employed to find one single nondominated solution per each optimization run.

Multi-objective genetic algorithms such as NSGA2 (Deb et al., 2002), on the other hand, find a set of optimal nondominated solutions in a single run without the need to convert the multi-objective problem into a single-objective problem. In order to identify nondominated solutions, NSGA2 uses a ranking selection method to emphasize the nondominated solutions, and a crowding distance method to maintain diversity in the solutions. The crowding distance method measures the density of the solutions in a specific region in the search space.
First, all individuals in a population are classified into several nondomination ranks based on a problem’s objectives. Within a given nondomination rank, NSGA also sorts the solutions according to their crowding distance. Then, NSGA2 uses the binary tournament selection method by picking two solutions from the population and:

- If one solution is feasible and the other solution is infeasible, NSGA2 selects the feasible solution
- If both solutions are infeasible, NSGA2 selects the one with smaller overall constraint violation
- If both solutions are feasible and they belong to different nondomination ranks, NSGA2 selects the solution with lower (better) rank
- If both solutions are feasible within the same nondomination rank, NSGA2 selects the solution that is located in a less crowded region

Afterwards, NSGA2 implements the regular genetic algorithm operators (crossover and mutation) on the selected solutions to create a new population. Note that NSGA2 handles the constraints within the aforementioned selection algorithm (Deb et al. 2002).

In this study, we use the NSGA2 source code for implementing the optimization model. The source code is accessible from [http://www.egr.msu.edu/~kdeb/codes.shtml](http://www.egr.msu.edu/~kdeb/codes.shtml).
5-2-4 Optimization model

5-2-4-1. Decision Variables

Two decision variables for each ASR well (in total 28 decision variables) are injection rate ($INJ^R_i$) and extraction duration ($EXT^D_i$). Here, injection duration ($INJ^D_i$) is equal to two months for all wells. While the injection rate of each well ($INJ^R_i$) is a decision variable, extraction rate ($EXT^R_i$) is a given value for each well because the JVWCD is not willing to change the settings of any installed pumps (written communication with JVWCD).

We model the injection rates as real variables from zero (no injection) to their specified maximum value (Equation 3). The maximum injection rate is proportional to the ability of the aquifer to accept the injectate. The JVWCD has estimated the wells maximum injection rate using injection tests (SLCWCD, 1996).

\[ 0 < INJ^R_i < INJ^R_{i, \text{MAX}} \quad \text{for } i = 1,2,\ldots,14 \]  

(3)

Extraction durations are modeled by eight discrete values of 0, 15, 30, 45,..., 105 days (Equation 4). To do so, we model them as binary variables using three bits with lower and upper bounds of 0 and 7. This produces exactly eight integer values of 0 to 7. Then, multiplying these integer values by 15 provides the extraction durations in unit of days.

\[ EXT^D_i = 0 \text{ or } 15 \text{ or } 30 \text{ or } \ldots \text{ or } 105 \text{ days} \quad \text{for } i = 1,2,\ldots,14 \]  

(4)
5-2-4-2- Objective functions

The first objective of the optimization model is to maximize the system’s overall REN (SYS\textsubscript{REN}):  

\[
\text{SYS}_{\text{REN}} = \text{Maximize} \frac{\sum_{i=1}^{14} (\text{REN}_i \times \text{INJ}_i^R \times \text{INJ}_i^D)}{\sum_{i=1}^{14} (\text{INJ}_i^R \times \text{INJ}_i^D)}  
\]  

(5)

Where the REN of each well (\textit{REN}_i) is a function of injection/extraction rates and durations. The ANN models with Equation 2 calculate \textit{REN}_i in each well.

The second objective is to minimize the total extracted water from the system within year 2 (SYS\textsubscript{EXT}):  

\[
\text{SYS}_{\text{EXT}} = \text{Minimize} \sum_{i=1}^{14} (\text{EXT}_i^R \times \text{EXT}_i^D)  
\]  

(6)

A simultaneous optimization of Equations 5 and 6 maximizes the system’s overall REN with the least amount of extraction within year 2.

The third objective is to minimize the system’s extraction cost within year 2 (SYS\textsubscript{COST}):  

\[
\text{SYS}_{\text{COST}} = \text{Minimize} C \times \sum_{i=1}^{14} (\text{EXT}_i^R \times \text{EXT}_i^D \times \text{Lift}_i)  
\]  

(7)

Where \textit{C} is the cost per unit pumping per length of hydraulic lift which is assumed equal to 0.002 \$/m^4, and \textit{Lift}_i is the difference between ground surface and water level in well \textit{i} during extraction. Because the wells' extraction rates are constant and the wells'
lift values reach a steady-state value within about one day, we assume the wells' $Lift_i$
unchanged considering the temporal resolution used in this study. The MNW2 package
used in the regional MODFLOW model computes wells' water levels. We assume
injection costs are the same for all wells, and therefore, Equation 7 only considers
extraction costs.

5-2-4-3- Model's constraint

In addition to the bounds imposed on decision variables (Equations 3 and 4), we
also exert a constraint in the optimization model. The model constraint enforces
injecting a given volume of surplus surface water (SURPLUS) into the system:

$$SYS_{INJ} \geq SURPLUS$$  \hspace{1cm} (8)

where $SYS_{INJ}$ is the volume of water injected to the system. Usually, ASR systems need to
impose an upper limit on water levels in wells to avoid water mounding during injection.
In this study, however, the maximum injection rate of each well has been determined
based on aquifer capacity for accepting the injectate. Therefore, we do not explicitly
consider a constraint regarding water mounding during injection. Nevertheless, the
regional MODFLOW model will be used to confirm that the highest water levels in the
wells are sufficiently below ground surface.
5-2-4-4- Optimization scenarios

To address the ASR system performance, we investigate two scenarios within the multi-objective optimization model:

Scenario 1) Simultaneous optimization of Equations 5 and 6. This scenario maximizes SYS\textsubscript{REN} with the least extraction volume from the system.

Scenario 2) Simultaneous optimization of Equations 5, 6, and 7. This scenario maximizes SYS\textsubscript{REN} with the least extraction volume and extraction cost.

The decision variable bounds (Equations 3 and 4) and the model constraint (Equation 8) are applied for both scenarios. In scenario 1, we explore three injection volumes (SURPLUS in Equation 8) of two, three, and four million cubic meters (Mm\(^3\)). The 4Mm\(^3\) SURPLUS is the maximum injection capacity of the JVWCD ASR system. Scenario 2 only addresses the 3Mm\(^3\) SURPLUS situation.

5-3- Results and discussion

In the following sections, we first present the computed wells' water levels using the regional MODFLOW model. Section 5-3-2 shows Scenario 1 results for the 3Mm\(^3\) SURPLUS situation. This section also provides the sensitivity analysis for NSGA2 parameters, demonstrates the superiority of NSGA2 over the E-constraint method, and displays the ANN models' accuracy by comparing their results with the regional MODFLOW-MT3DMS simulation. Section 5-3-3 compares Scenario 1 results for three tested SURPLUS values (2, 3, and 4Mm\(^3\)), and presents the wells' rankings based on this
scenario. Section 5-3-4 shows Scenario 2 results, and updates the wells’ rankings after considering pumping costs. Finally, Section 5-3-5 provides an operational guideline for the JVWCD ASR system.

5-3-1- Water levels in wells during ASR operations

Table 5-1 presents water elevations inside the wells computed by the regional MODFLOW model with the MNW2 package. Highest water elevations during injection were computed using the maximum injection rate of each well. Although the computed highest water elevations do not consider the additional water level rise that might occur from clogging (Pyne, 1995, page 119), for all wells, highest water elevation is well below the ground surface elevation. Therefore, in this study we assume that we will not encounter water mounding, if respecting the specified maximum injection rates. Table 5-1 also shows the hydraulic lifts for the specified extraction rate of each well. The lift values are used in Equation 7 to compute pumping costs.

5-3-2- Optimization scenario 1 with SURPLUS of 3 Mm³

5-3-2-1- Objective values and constraint

Scenario 1 employs two objectives via Equations 5 and 6. Equation 5 maximizes the system’s overall REN while Equation 6 minimizes the extraction volume within year 2. Equations 5 and 6 conflict with each other because as the extraction within year 2 increases, more injectate is recovered, and therefore, the system’s REN increases. Here,
Table 5-1. Using MNW2 package to compute water levels in wells during ASR operations

<table>
<thead>
<tr>
<th>Well name</th>
<th>Ground surface elevation (m)</th>
<th>Highest water elevation during injection (m)</th>
<th>Water elevation during extraction (m)</th>
<th>Lift (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLC3</td>
<td>1425</td>
<td>1323</td>
<td>1316</td>
<td>109</td>
</tr>
<tr>
<td>SLC4</td>
<td>1396</td>
<td>1320</td>
<td>1305</td>
<td>91</td>
</tr>
<tr>
<td>SLC5</td>
<td>1390</td>
<td>1321</td>
<td>1305</td>
<td>85</td>
</tr>
<tr>
<td>SLC6</td>
<td>1371</td>
<td>1319</td>
<td>1304</td>
<td>67</td>
</tr>
<tr>
<td>SLC8</td>
<td>1358</td>
<td>1324</td>
<td>1291</td>
<td>68</td>
</tr>
<tr>
<td>SLC9</td>
<td>1368</td>
<td>1316</td>
<td>1309</td>
<td>59</td>
</tr>
<tr>
<td>SLC15</td>
<td>1427</td>
<td>1317</td>
<td>1312</td>
<td>115</td>
</tr>
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<td>1319</td>
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</tr>
<tr>
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<td>1444</td>
<td>1321</td>
<td>1316</td>
<td>128</td>
</tr>
<tr>
<td>SLC28</td>
<td>1475</td>
<td>1338</td>
<td>1312</td>
<td>163</td>
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<td>SLC32</td>
<td>1408</td>
<td>1319</td>
<td>1304</td>
<td>104</td>
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<tr>
<td>SLC33</td>
<td>1460</td>
<td>1337</td>
<td>1268</td>
<td>192</td>
</tr>
<tr>
<td>SLC36</td>
<td>1430</td>
<td>1321</td>
<td>1301</td>
<td>129</td>
</tr>
<tr>
<td>SLC37</td>
<td>1379</td>
<td>1321</td>
<td>1295</td>
<td>84</td>
</tr>
</tbody>
</table>

we run the NSGA2 model with population size of 200 for 200 generations. Figure 5-2 shows 195 solutions with nondomination rank 1 (the best rank) in the last generation. Five solutions in the last generation belong to rank 2 and are dominated by the solutions in rank 1. Consequently, these dominated solutions are ignored.

Figure 5-2 shows that extracting the same volume as injection (3Mm$^3$) achieves REN of about 55%. None of the solutions in the nondominated (or Pareto) curve are absolutely better than others. Therefore, any solution in the nondominated set might be an acceptable solution. Herein, however, we are interested only in the solutions with REN more than 60%. Figure 5-2 shows 109 solutions with REN more than 60% with bigger blue circles.
Figure 5-2. System’s extracted water versus system’s REN in Scenario 1 with SURPLUS of 3 Mm³. Bigger blue circles show solutions with REN more than 60%.

NSGA2 tries to find the solutions that either satisfy the constraint (Equation 8) or have the least amount of constraint violation. Figure 5-3 shows that most solutions provide injectate of about 3Mm³ to the system.

5-3-2-2 Optimal decision variables

Because we have many optimal solutions, in order to present the range of changes for optimal decision variables (injection rates and extraction durations), we use
Figure 5-3. Capability of NSGA2 to satisfy the constraint of injecting 3Mm3 to the system

Box-and-whisker plots, or simply boxplots. Boxplots provide an easy way for presenting the data spread and consist of a box and two whiskers that are vertically extended from the box. The bottom and top of the box shows the first quartile (25th percentiles) and third quartile (75th percentiles), and the thicker line inside the box shows the second quartile or median. Whiskers represent the data outside the middle 50%. Some boxplots (including the one used in this study) also show outliers beyond the whiskers with individual points. Boxplots in Figures 5-4 and 5-5 show the range of optimal injection rates and extraction durations for 109 solutions with REN more than 60%. The dashed red lines in Figure 5-4 show the maximum allowed injection rate for each well.
Figure 5-4. Boxplots showing the range of optimal injection rates for each well in Scenario 1 with 3Mm3 SURPLUS. The red dashed lines show the maximum injection rates.

For some wells, we virtually do not see a box for injection rates or extraction durations—we only see the thicker median line. This implies that the range of changes in those variables is very small and most values are very close to each other. For example, injection rates and extraction durations are zero for wells SLC3, SLC15, SLC18, SLC22, and SLC28. For the remaining nine wells, the boxes cover the middle 50% of the data. For these nine operational wells and for the solutions with REN more than 60%,
Table 5-2 shows representative decision variables for each well considering the mean of injection rates and the median of extraction durations. We use the median of extraction durations because of the discrete nature of this variable.

Figure 5-5. Boxplots showing the range of optimal extraction durations in Scenario 1 with 3Mm3 SURPLUS

Most wells require extracting approximately two times their injection volume (see column 7 in Table 5-2). The wells SLC4 and SLC33, however, need a higher ratio of extraction to injection volumes. This occurs because among the nine wells in Table 5-2,
SLC4 has the highest gradient and SLC33 has the largest value of total transmissivity. Larger values of gradient and transmissivity result in higher groundwater velocity. Higher groundwater velocity allows the injectate to travel further from the well’s capture zone during the storage duration, and therefore, more extraction is required to recover the injectate (Forghani and Peralta, 2017a).

Table 5-2. Representative decision variables for nine operational wells in Scenario 1 with 3Mm3 SURPLUS

<table>
<thead>
<tr>
<th>Well name</th>
<th>Inj rate mean (m3/d)</th>
<th>Inj volume (Mm3)</th>
<th>Ext rate (m3/d)</th>
<th>Ext duration median (day)</th>
<th>Ext volume (Mm3)</th>
<th>Ratio of Ext/Inj volumes</th>
<th>REN (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLC 4</td>
<td>7950</td>
<td>0.48</td>
<td>23980</td>
<td>60</td>
<td>1.44</td>
<td>3.0</td>
<td>79.9</td>
</tr>
<tr>
<td>SLC 5</td>
<td>4550</td>
<td>0.27</td>
<td>7830</td>
<td>75</td>
<td>0.59</td>
<td>2.2</td>
<td>87.7</td>
</tr>
<tr>
<td>SLC 6</td>
<td>2840</td>
<td>0.17</td>
<td>7100</td>
<td>45</td>
<td>0.32</td>
<td>1.9</td>
<td>88.0</td>
</tr>
<tr>
<td>SLC 8</td>
<td>4040</td>
<td>0.24</td>
<td>11010</td>
<td>45</td>
<td>0.50</td>
<td>2.0</td>
<td>99.0</td>
</tr>
<tr>
<td>SLC 9</td>
<td>1830</td>
<td>0.11</td>
<td>4160</td>
<td>45</td>
<td>0.19</td>
<td>1.7</td>
<td>90.7</td>
</tr>
<tr>
<td>SLC 32</td>
<td>8050</td>
<td>0.48</td>
<td>24250</td>
<td>45</td>
<td>1.09</td>
<td>2.3</td>
<td>79.4</td>
</tr>
<tr>
<td>SLC 33</td>
<td>7340</td>
<td>0.44</td>
<td>21800</td>
<td>75</td>
<td>1.64</td>
<td>3.7</td>
<td>87.5</td>
</tr>
<tr>
<td>SLC 36</td>
<td>8070</td>
<td>0.48</td>
<td>24250</td>
<td>45</td>
<td>1.09</td>
<td>2.3</td>
<td>76.0</td>
</tr>
<tr>
<td>SLC 37</td>
<td>4970</td>
<td>0.30</td>
<td>14660</td>
<td>45</td>
<td>0.66</td>
<td>2.2</td>
<td>98.5</td>
</tr>
<tr>
<td>Overall</td>
<td>2.98</td>
<td></td>
<td></td>
<td></td>
<td>7.51</td>
<td>2.5</td>
<td>85.3</td>
</tr>
</tbody>
</table>

5-3-2-3- Sensitivity of NSGA2 parameters

The NSGA2 input parameters are population size, number of generations, probability of mutation and crossover (for both real and binary variables), and distribution indexes for crossover and mutation of real variables (Deb et al., 2002). We use 20 as the value for distribution indexes for crossover and mutation of real variables.
Also, we use the crossover probability of 0.8 for both real and binary variables. We perform sensitivity analyses for mutation probability (for both real and binary variables), population size, and the number of generations.

Figure 5-6 shows that there is not a considerable improvement in the Pareto curve (for a given extraction volume we do not achieve a significantly higher REN) for population size and number of generations beyond 100. Nevertheless, we present all results in this study from NSGA2 runs with population size and number of generations of 200.

Figure 5-6. Sensitivity analysis on the values of population size (P) and generations number (G)
The recommended value for mutation probability of real variables is one divided by the number of real variables (14) which equals 0.07 (Deb et al., 2002). Sensitivity analysis, however, showed that using the value of 0.15 provides better results—higher RENs for a given extraction volume. The recommended value for mutation probability of binary variables is one divided by the total number of bits (14x3=42) which equals 0.02 (Deb et al., 2002) Sensitivity analysis confirmed that this value achieves better results than the tested values of 0.005, 0.01 and 0.04. Therefore, all results in this study are from NSGA2 runs with a real-variable mutation probability of 0.15 and a binary-variable mutation probability of 0.02.

5-3-2-4- Comparing multi-objective optimization with E-constraint technique

Figure 5-7 compares the results of the NSGA2 model with the E-constraint method. The four red triangles in this figure are the optimal solutions obtained from four separate single-objective optimizations by constraining the total extraction volume to the values of 5, 7.4, 9.9, and 11.1Mm³. Each run of the E-constraint method tries to find the system's maximum achievable REN for the imposed extraction volume constraint.

The superiority of the NSGA2 lies in the fact that it addresses all objectives simultaneously without requiring water managers to perform the challenging task of converting the objectives into a single objective. In addition, NSGA2 develops the Pareto optimal solutions in a single run. Table B-1 in Appendix B reports the optimal wells'
injection rates and extraction durations for the four optimal solutions shown in Figure 5-7.

Figure 5-7. Superiority of the NSGA2 over E-constraint method to provide a set of optimal solutions in a single run

5-3-2-5- Confirming the accuracy of the ANN models

Forghani and Peralta (2017b) report the high accuracy of the ANN models for estimating REN in fully penetrating ASR wells screened in one-layer systems. In this section, we present the accuracy of using the ANN models with Equation 2 to estimate REN for partially penetrating wells screened in multiple strata.
For two tested strategies (including the strategy in Table 5-2), the error in overall REN is less than 1% while the maximum individual REN error is 7.7% (for well SLC33). Figure 5-8 compares the ANNs results with a MODFLOW-MT3DMS run for the strategy shown in Table 5-2. The figure displays the reliability of using the ANNs with Equation 2 for estimating REN in multi-layer wells. For the Table 5-2 strategy, the MODFLOW-MT3DMS simulation run time is about four hours. This further reveals the crucial importance of using the developed neural networks in studies that require many REN simulations (e.g. optimization and uncertainty analysis).

![Figure 5-8. Comparison between the results of the ANNs and a MODFLOW-MT3DMS simulation](image)

Also, the MODFLOW-MT3DMS simulation results show that if we spread the injection volume over three months (instead of two months), the change in REN values are negligible.
5-3-3- Optimization Scenario 1 with SURPLUS values of 2 and 4 Mm$^3$

This section compares Scenario 1 results for three tested SURPLUS values of 2, 3, and 4 Mm$^3$. Comparing the optimal decision variables between these three situations enables ranking the wells based on their recovery effectiveness.

Figures 5-9 and 5-10 present the optimal injection rates and extraction durations for solutions with REN more than 60% for the 4 Mm$^3$ SURPLUS situation. Figure 5-9 shows that the nine operational wells in the 3 Mm$^3$ SURPLUS situation (Table 5-2) now have even higher injection rates, which are close to their maximum injection capacity. In order to increase the system’s injectate and satisfy the 4 Mm$^3$ SURPLUS constraint, the wells SLC3, SLC15 and SLC18 also receive some injectate (SLC18 actually receives injectate close to its maximum capacity). However, NSGA2 suggests short extraction durations for these wells, especially for wells SLC3 and 15, which have virtually zero extraction durations (Figure 5-10). This occurs because wells SLC3 and 15, which are located in high-gradient areas, cannot recover any injectate after one year of storage. Therefore, the NSGA2 model assigns zero extraction to these wells because extracting from these wells would negatively impact one objective (the system’s extraction volume) without any improvement for the other objective (the system’s REN). More injection to other wells is beneficial to maximize the system’s REN in the 4 Mm$^3$ SURPLUS situation, and therefore, NSGA2 suggests the highest allowed injection rates for the nine operational wells in the 3 Mm$^3$ SURPLUS situation.
Figure 5-9. Boxplots showing the range of optimal injection rates in Scenario 1 with 4Mm³ SURPLUS. The red dashed lines show the maximum injection rates.

Again, wells SLC22 and 28 receive zero injection, and this suggests that the wells SLC3, SLC15, SLC22, and SLC28 are the worst wells in the system to which no water should be injected for a yearly storage. We categorize these wells as the wells with Rank 3. Among the five un-operational wells in the 3Mm³ SURPLUS situation, Figure 5-9
Figure 5-10. Boxplots showing the range of optimal extraction durations in Scenario 1 with 4Mm3 SURPLUS

shows that SLC18 receives injectate as much as its capacity, therefore, we can categorize this well as an average well with Rank 2.

Similar to the optimal decision variable for the 3Mm³ SURPLUS situation (Figures 5-4 and 5-5), the optimal decision variables for the 2Mm³ situation (not shown graphically) show that wells SLC5, 6, 8, 9, 36, and 37 are again the wells with high injections. Therefore, we can categorize these wells as the best wells in the system with
Rank 1. However, in addition to the five un-operational wells in the 3Mm$^3$ SURPLUS situation (wells SLC3, 15, 18, 22, 28), the results of the 2Mm$^3$ SURPLUS situation suggest significantly less injectate (and short extraction duration) for wells SLC4, 32, and 33. This implies that we can also consider these three wells as average wells with Rank 2—NSGA2 suggests utilizing these wells only if injecting more than the capacity of the Rank 1 wells is required. Table 5-3 shows the JVWCD wells’ rankings based on their recovery effectiveness (REN) for a yearly storage of injected water.

Table 5-3. The JVWCD wells’ rankings based on Scenario 1

<table>
<thead>
<tr>
<th>Rank 1 (Best)</th>
<th>Rank 2 (Average)</th>
<th>Rank 3 (Worst)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLC5, SLC6, SLC8, SLC9, SLC36, SLC37</td>
<td>SLC4, SLC18, SLC32, SLC33</td>
<td>SLC3, SLC15, SLC22, SLC28</td>
</tr>
</tbody>
</table>

Figure 5-11 shows the Pareto curves obtained for the three tested SURPLUS situations. This figure indicates that as the injection to the system during year 1 increases, more extraction during year 2 is required to achieve a given REN. This occurs because increasing the injection to the system requires utilizing some of the wells with Ranks 2 or 3. This is crucial especially if the volume of surplus water is such high that it enforces injecting to the wells with Rank 3 (because little injectate can be recovered from these well).
5-3-4- Optimization Scenario 2

Scenario 2 addresses the objectives in Equations 5 to 7 simultaneously—maximizing REN while minimizing extracted volume and pumping cost. We examine this scenario only for the 3Mm³ SURPLUS situation.

![Figure 5-11. Pareto solutions for SURPLUS values of 2, 3, and 4 Mm³](image)

Optimal decision variables in this scenario are comparable to Figures 5-4 and 5-5 except for well SLC33. This well has the highest lift value (Table 5-1), and therefore, Scenario 2 suggests little extraction from this well. Accordingly, this well receives little injectate. This degrades this well to Rank 3. Other wells still follow the rankings in Table 5-3. Table 5-4 presents the wells' rankings based on Scenario 2.
Table 5-4. The JVWCD wells’ rankings based on Scenario 2

<table>
<thead>
<tr>
<th>Rank 1 (Best)</th>
<th>Rank 2 (Average)</th>
<th>Rank 3 (Worst)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLC5, SLC6, SLC8, SLC9, SLC36, SLC37</td>
<td>SLC4, SLC18, SLC32</td>
<td>SLC3, SLC15, SLC22, SLC28, SLC33</td>
</tr>
</tbody>
</table>

Figure 5-12 shows the three objective values of Scenario 2 using the 124 solutions with REN more than 60%. For illustration, the Pareto curve in Figure 5-2 is also redrawn to compare the results between the two scenarios. This figure shows that in order to address the new objective of minimizing the pumping cost, Scenario 2 provides slightly less RENs for given extraction volumes, especially for solutions with REN more than 80%. Table B-2 in Appendix B shows the optimal wells’ injection rates and extraction durations for four selected solutions in Scenario 2.
5-3-5- Operational guidelines

We employ the wells’ rankings to suggest an operational guideline for the JVWCD for a condition where there is no need to extract water in the same year of injection (injectate yearly storage). The operational guideline for this condition is:

- Rank 1 wells are always the first wells that should be utilized
- If SURPLUS values exceed the capacity of Rank 1 wells, Rank 2 wells should be utilized
- There is no benefit of utilizing Rank 3 wells in this condition

The results in Sections 5-3-2 to 5-3-4 and the above guidelines address the system for a condition where there is no extraction in year 1 (the same year as injection). On the other hand, as mentioned, Forghani and Peralta (2017c) investigated this ASR system for the other extreme condition, where there is a significant amount of extraction in year 1, and showed that most wells can achieve REN more than 90% by extracting three times their injection volume.

The results obtained from the aforementioned extreme conditions can also be used to present an operational guideline for the conditions where there is a need to extract some water in year 1. For example, while the results presented in this study show that the Rank 3 wells (i.e. wells SLC3, 15, 22, and 28) should have zero injection for yearly storage condition, this implies that the JVWCD should either avoid injecting into them, or extract from these wells (preferably three times their injection volume) in the same year of injection. Both cases satisfy zero injectate for yearly storage in these wells.
Therefore, the operational guideline for the conditions where in addition to extraction in year 2, some extractions are also required in year 1 is:

- Rank 1 wells are always the first wells that should be utilized
- If SURPLUS values exceed the capacity of Rank 1 wells (but less than the capacity of both Rank 1 and 2 wells), Rank 2 wells should be utilized. Here, Rank 2 wells should be used for extraction in year 1 (up to three times of their injection)
- If SURPLUS values exceed the capacity of the wells with Ranks 1 and 2, Rank 3 wells can also be utilized (after utilizing the wells with Ranks 1 and 2). Here, Rank 3 wells are the first wells that should be used for extraction in year 1 (up to three times of their injection)

5-4- Conclusion

We use a multi-objective genetic algorithm model to derive a set of optimal solutions addressing the performance of an ASR system in a freshwater aquifer. Recovery effectiveness (REN) is the performance index of the studied ASR system, which equals the injectate proportion that the same wells can recover. The study addresses the system’s REN for the conditions of injecting within year 1 and extracting within year 2 (after 12 months of water storage in the aquifer).

The optimization model employs generalized neural networks for estimating REN. This allows performing many REN simulations in the optimization model. Post-optimization evaluation of ANN-computed RENs using a regional multi-layer MODFLOW-
MT3DMS model presents the high accuracy of the ANNs for estimating REN even for partially penetrating wells screened in multiple layers. Therefore, this paper introduces the generalized neural networks as a valuable tool for estimating REN for many ASR systems worldwide.

Three considered objectives are 1) maximizing the system’s overall REN, 2) minimizing the system’s extraction volume within year 2, and 3) minimizing pumping costs. The optimization model with objectives 1 and 2 generates Pareto solutions representing the trade-offs between the system’s extracted volume and the system’s achievable REN. The optimization model with objectives 1 to 3 finds the optimal solutions that maximize the recovery of the year 1 injected water with the least extraction volume and cost within year 2.

Comparing the optimal decision variables (i.e. the wells' optimal injection rates and extraction durations) for three tested injectate volumes enables categorizing the wells into three rankings based on their recovery effectiveness. Finally, we use the wells' rankings to suggest operational guidelines to maximize the performance of the studied ASR system. The study presents the efficiency of using the generalized neural networks with multi-objective genetic algorithms for evaluating the performance of ASR systems in freshwater aquifers.
References


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CHAPTER 6
CONCLUDING REMARKS AND FUTURE WORK

6-1- Summary and conclusions

This dissertation employs simulation, statistical, and optimization models to evaluate the performance of an Aquifer storage and recovery (ASR) system in a fresh water aquifer (FWA) in Utah. ASR involves artificially recharging an aquifer through well(s) using surplus water for later recovery in high-demand months. The operators of the studied ASR system developed this ASR system as a means of receiving additional water rights to supplement their pre-existing water rights for extraction in dry months. However, the region's water regulators define the performance of this ASR system as the amount of the injected water that is recoverable from the same wells during extraction periods. The study proposes recovery effectiveness (REN) as the performance index of this ASR system. REN equals the injectate proportion that the same wells can recover. Quantifying the system's achievable REN is required to determine the amount of the additional water rights. Similarity between the injected water and native groundwater, however, prevents an accurate REN estimation using on-field techniques. This necessitates the use of modeling for estimating REN in this system.

Chapter 2 presents a methodology employing MODFLOW and MT3DMS, two commonly used models for flow and contaminant transport simulations, to estimate REN. In order to distinguish the injected water from native groundwater, the transport model (MT3DMS) assumes an imaginary non-reactive contamination in the injected water. MT3DMS tracks the
movement of the injected "contamination" during an ASR operation. The estimated REN equals the proportion of the injected "contamination" that the same ASR well can recover.

Chapter 2 also presents the crucial importance of model horizontal discretization on computed REN. Background seepage velocity, the seepage velocity before beginning ASR operation, is the main criterion affecting REN in the studied ASR system. Accordingly, the study’s results show that screening in less permeable layers, as long as it does not hamper the functionality of the ASR well during injection and extraction, can improve REN. In addition, the importance of avoiding screening in higher permeability layers increases as the background gradient increases. Therefore, this chapter introduces vertical heterogeneity as a crucial factor on the performance of ASR systems in FWA.

Chapter 3 presents a software for a rapid REN prediction without the need to prepare and run MODFLOW-MT3DMS models. The software invokes two trained artificial neural networks (ANN) as surrogate simulators. The developed software also allows conducting sensitivity analysis of different factors that can affect REN. Therefore, the software can help to identify superior hydrogeological or operational settings instantly. The software is applicable not only for the studied ASR system, but for any other ASR system whose parameters are within the range of values used to develop the ANNs.

As an example, Figure 3-10 shows a screenshot of the software developed in Chapter 3. The figure presents the mutual impacts of injection rate and extraction rate on REN_90d (achievable REN after extracting for 90 days) for the condition of 1-year storage of the injected water. The figure has been obtained from a number of ANN simulations by changing the values
of injection rates and ratio of extraction to injection rates (E/I) in their specified range, while keeping the other independent variables (i.e. hydraulic conductivity, porosity, aquifer thickness, and background gradient) constant. Figure 3-10 shows that an injection rate more than 7000 m$^3$/d and an E/I more than 2.5 (i.e. extraction rate more than 17,500 m$^3$/d) is needed to achieve a REN$_{90d}$ more than 90% for the examined ASR well after one year storage of injected water.

Chapter 4 shows that most of the final achievable REN (REN after five years of operation), occurs while extracting three times the injection volume (by achieving REN$_{RATIO3}$), and that further extraction cannot significantly increase REN. After extracting three times the injection volume, the injectate either has been captured by the well, or has departed the well's capture zone. Therefore, REN$_{RATIO3}$ is a reasonable approximation of the final REN in this system.

The results also show that the system's overall REN is more than 95% if the wells extract three times their injection volume in the same year of injection (typically within 3-4 months after injection). This is feasible due to pre-existing groundwater pumping rights in the studied ASR system. Extracting merely the same volume as injectate would achieve REN not more than 75% for most wells. This highlights the importance of having pre-existing water rights to achieve a high REN.

Chapter 4 also employs the multivariate adaptive regression splines (MARS) regression technique to statistically analyze the studied ASR system for the current operational scheme. MARS identifies background hydraulic gradient and hydraulic conductivity (or background Darcian velocity) as the most significant parameters affecting REN in the studied system. MARS
finds threshold values within significant variables spaces and presents equations for estimating REN within each section of each significant variable space. For instance, MARS suggests that hydraulic conductivity (K) can negatively impact REN (with a specified coefficient) only for the wells with K more than 20m/d. MARS results also demonstrate that maximizing REN requires utilizing the wells located in areas with background Darcian groundwater velocities less than 0.03m/d.

Chapter 5 employs optimization models to identify the optimal wells for a yearly storage of the injected water—Injecting within year 1 and extracting within year 2. The addressed objectives are 1) maximizing the system’s overall REN, 2) minimizing the system’s extraction volume within year 2, and 3) minimizing pumping costs. These objectives maximize the system’s REN with the least amount of extraction volume and extraction cost. The optimization model results also identify the best, average, and worst wells in the system. Table 5-4 presents the rankings of the 14 wells in the studied ASR system by considering the objectives 1 to 3 simultaneously. The results also show that as the injection to the system during year 1 increases, more extraction during year 2 is required to achieve a given REN. This occurs because increasing the injection to the system requires utilizing some of the wells with Ranks 2 or 3.

For estimating REN, the optimization model in Chapter 5 employs the ANNs developed in Chapter 3. Using the ANNs as the surrogate simulator of a transport simulation is vital because the optimization model requires performing many REN simulations. In addition, post-optimization evaluation of ANN-computed RENs using a regional multi-layer MODFLOW-MT3DMS model presents the high accuracy of the ANNs for estimating REN. Therefore, while
Chapter 3 presents the high accuracy of the ANNs for estimating REN in fully penetrating ASR wells screened in one-layer systems, Chapter 5 introduces the ANNs as a valuable tool to estimate REN in many ASR systems worldwide, even for partially penetrating wells screened in multiple strata.

6-2- Future works

As mentioned, the JVWCD tried extensive tracer tests to track the injected water and quantify the REN, but the results were uncertain and inaccurate because of the similarity between the injected water and native groundwater. This causes reliance on groundwater models to estimate REN. However, it is absolutely beneficial to acquire reliable field data to calibrate the groundwater models. More advanced tracer tests should be designed to have a more accurate estimation of REN for comparison with the models results.

Also, in order to improve the generalization of the developed ANNs in Chapter 3, more simulations can be implemented to further broaden the range of independent variables, especially regarding hydraulic conductivity.
APPENDICES
Appendix A

We use the USGS MODTMR code (Leake and Claar 1999) to prepare both refined mesh input files and specified boundary data for the TMR model. To produce Figure 2-4a, we use TMRDIFF (Leake and Claar 1999), an accompanying code with MODTMR, to compare the heads at the boundary cells of TMR model with the heads in the corresponding area of the regional model. We use ModelMuse (Winston 2009) to prepare refined mesh input files of LGR models from the TMR model. We prepare the specified head boundaries for LGR models using the MODFLOW-LGR2 code (Mehl and Hill 2013).

The BFH2 package of MODFLOW-LGR2 (Mehl and Hill 2013) runs an LGR model independently (without the need to run the rest of the TMR model) after preparing its specified head boundaries via two-way TMR and LGR model coupling. Note that we implement grid refinements after modeling the desired scenario of ASR operation (Table 2-1) in the regional model. No new significant stress should be applied on local TMR or LGR models. If a new stress is applied on the LGR models, the BFH2 package enables identifying the validity of the boundaries for the new stress. For example, we initially obtained the specified head boundaries of the vertically refined LGR model for Scheme A in Figure 2-7. We used the same boundaries for screen schemes B, C, and D. The results of the BFH2 package (written at the end of the Modflow listing file) confirmed the validity of using the boundaries for new schemes.

Using the TMR technique for the first refinement stage has another advantage for preparing computationally efficient models for SLC8. SLC8 is open in regional model layers 6 and 7, which is the deepest part of principal aquifer. The pumping in these layers has little
effect on shallow unconfined and confining units modeled by layers 1 and 2 of the regional model. To decrease run time, it is advantageous to remove layers 1 and 2 (while representing their effect on layer 3 by using specified flux boundaries). Unlike the current version of MODFLOW-LGR2 code, MODTMR has the capability of removing layers 1 and 2. So, we create TMR model by removing layers 1 and 2 of regional model (see Figure 2-3). Therefore, all the refined models (TMR and LGR models) for SLC8 only simulate the principal aquifer.

MODTMR prepares the input files of the TMR model based on the MODFLOW 96 version. For use in MODFLOW-LGR2 code, we need to convert the dataset of the TMR model into the MODFLOW 2005 version. Furthermore, we change two of the packages used with the MODFLOW 2005 version of the TMR model. First, we use the revised multi-node well (MNW2) package (Konikow et al. 2009) to simulate the multinode ASR well. Neville and Tonkin (2004) show that using the MNW2 package is the most accurate method to simulate multinode wells penetrating more than one layer of a model. Second, we modify the TMR model by replacing the original block-centered flow (BCF) package with the layer property flow (LPF) package. This helps to obtain more accurate aquifer properties for the vertically refined LGR model during input data preparation by ModelMuse. The differences in model results between the original MODFLOW 96 version of the TMR model and the modified MODFLOW 2005 version for use in LGR implementation are negligible.

Figure A-1 compares the computed head at the ASR well between the regional model, the TMR model, and the most refined LGR model (3rd LGR model in Table 2-2). The accuracy in computing the ASR well head changes increases by preparing more refined TMR and LGR
models. The MNW2 package in the LGR model provides additional accuracy in computing the head at the wellbore considering the effects of aquifer loss using the specified well radius. Due to having a very large cell size, the regional model computes head changes in the ASR well very poorly. The computed heads shown for the regional model are interpolated heads at the actual location of the ASR well within the regional model cell. All TMR and LGR models have mass balance errors well below 1%.

Figure A-1-Computed head at ASR well using different flow models
## Appendix B

**Table B-1. Optimal decision variables for four solutions in Scenario 1 with 3Mm3 SURPLUS**

<table>
<thead>
<tr>
<th>Well name</th>
<th>Inj rate, m³/d</th>
<th>Ext Dur, day</th>
<th>Inj rate, m³/d</th>
<th>Ext Dur, day</th>
<th>Inj rate, m³/d</th>
<th>Ext Dur, day</th>
<th>Inj rate, m³/d</th>
<th>Ext Dur, day</th>
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<tr>
<td>SLCWCD4</td>
<td>8167</td>
<td>30</td>
<td>7998</td>
<td>45</td>
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<td>0</td>
<td>8156</td>
<td>105</td>
</tr>
<tr>
<td>SLCWCD5</td>
<td>5454</td>
<td>90</td>
<td>5456</td>
<td>105</td>
<td>5455</td>
<td>105</td>
<td>4888</td>
<td>105</td>
</tr>
<tr>
<td>SLCWCD6</td>
<td>3801</td>
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### Table B-2. Optimal decision variables for four solutions in Scenario 2 with 3Mm³ SURPLUS

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CURRICULUM VITAE

Ali Forghani

Phone: (626) 298-4319   Email: Ali_Forghaani@yahoo.com

EDUCATION

PhD, Civil Engineering-Water Resources Engineering, Utah State University, Dec 2017
M.Sc., Civil Engineering-Water Resources Engineering, Sharif University of Technology, Tehran, Iran, Oct 2007
B.Sc., Civil Engineering, Isfahan University of Technology, Isfahan, Iran, Aug 2005

RESEARCH INTERESTS
- Groundwater flow and contaminant transport modeling
- Heuristic optimization models
- Machine learning and data analysis
- Hydrologic modeling

RESEARCH EXPERIENCES
- “SIMULATION AND OPTIMIZATION MODELS TO EVALUATE PERFORMANCE OF AQUIFER STORAGE AND RECOVERY WELLS IN FRESH WATER AQUIFERS”, PhD dissertation
- Proposed the new Recovery Effectiveness (REN) index to quantify performance of aquifer storage and recovery (ASR) systems in freshwater aquifers (FWA)
- Employed groundwater flow model (MODFLOW) and transport simulations (MT3DMS) to quantify REN
- Implemented a two stage grid refinement technique using TMR and LGR to prepare a refined (both horizontally and vertically) flow model for an accurate transport modeling
- Results revealed the crucial effect of aquifer heterogeneity on REN in FWA
- Employed Multivariate Adaptive Regression Splines (MARS) and multiple linear regression to evaluate the overall performance of an ASR system with 14 wells in a FWA in Utah
- Developed Artificial Neural Networks (ANN) in R programming language as a generalized REN predictor in FWA
- Wrote C++ MPI code to run in parallel a large number of MODFLOW-MT3DMS simulations to prepare the dataset needed for training the ANN models
- Developed a Graphical User Interface (GUI) using Python language to facilitate using the ANN models and to perform sensitivity analysis and stochastic modeling of different factors affecting REN
- Wrote C++ code to implement Genetic Algorithms for optimizing REN in an ASR system subject to physical and technical constraints

• “CONJUNCTIVE USE OF SURFACE AND GROUND WATER RESOURCES IN ARID REGIONS”, M.Sc thesis
- Employed Modflow and Genetic Algorithms (in MATLAB) for an optimal use of water resources in an arid region with the need of transferred water from neighboring basins
- Results found an annual increase of 40% in the amount of imported surface water is needed in order to meet all the demands with negligible drop in the aquifer’s level.

PUBLICATIONS


Abolfazl Shamsai and Ali Forghani, “Conjunctive use of surface and ground water resources in arid regions,” Iranian Water Resources Research, 2011, volume 7, number 2; Page(s) 26 to 36

Ali Forghani and Richard C. Peralta, “Performance Assessment of Aquifer and Storage Recovery Wells in Freshwater Aquifers: Predominant Importance of Background Hydraulic Gradient”, In process

Ali Forghani, Richard C. Peralta, "Intelligent Performance Evaluation of ASR systems in Freshwater Aquifers", In process

CONFERENCES


TEACHING EXPERIENCE

- Instructor, Utah State University, Logan, Utah [2012-2014]
  Developed curriculum in all areas including instruction, grading, preparing tests (quizzes, midterms, finals), holding office hours, and assigning final grades for half of the course related to surface water
  - "Hydrologic modeling", (3 semesters)

- Grader, Utah State University, Logan, Utah [2012-2014]
  Graded for half of the course related to groundwater
  - "Hydrologic modeling", (3 semesters)

- Instructor, Taft Azad University, Yazd, Iran [2008-2010]
  Developed curriculum in all areas including instruction, grading, preparing tests (quizzes, midterms, finals), holding office hours, and assigning final grades
  - "Water and wastewater engineering", (4 semesters)
  - "Fluid mechanics", (3 semesters)

- Instructor, Ardakan Azad University, Yazd, Iran
- [2009-2010] Developed curriculum in all areas including instruction, grading, preparing tests (quizzes, midterms, finals), holding office hours, and assigning final grades
  - "Water and wastewater engineering", (2 semesters)
  - "Water and wastewater engineering project", (2 semesters)
  - "Fluid mechanics", (2 semesters)
  - "Water structures", (2 semesters)

PROFESSIONAL EXPERIENCE

Hydrogeologist, Yazd Regional Water Corp, Yazd, Iran [2008-2010]
  - Prepared water related GIS maps for Yazd Province
  - Reviewed and evaluated the quality of groundwater related studies implemented by consulting companies

Structural Engineer, Civil Engineering office No. 80, Yazd, Iran [2007-2009]
  - Designed the structure (using ETABS and SAFE) and prepared corresponding structural drawing (using AUTOCAD) of seven residential and commercial buildings in Yazd, Iran
  - Supervised construction of four residential buildings in Yazd, Iran

Structural Engineer, Tehran, Iran [2007-2008]
  - Designed the structure of telecommunications towers in Tehran, Iran (Using SAP and SAFE)

TECHNICAL EXPERTISE

General: C++, Python, R, FORTRAN, MATLAB, ArcGIS, GAMS, LINGO, and MPI (for parallel programming)

Water Engineering: Modflow-2005, MODPATH, Modflow–LGR2, Modflow-USG, MT3DMS, Modflow GUIs (e.g. GWV, GMS, and ModelMuse), HEC-HMS, and EPANET

Structural Engineering: ETABS, SAP, SAFE, and AutoCAD
PERMISSIONS

Title: Transport modeling and multivariate adaptive regression splines for evaluating performance of ASR systems in freshwater aquifers

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Publication: Journal of Hydrology
Publisher: Elsevier
Date: October 2017
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