Aquifer Parametrization and Evaluation of Dipole Flow in Recirculation Wells

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Thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Department of Civil and Environmental Engineering in the Graduate School of Duke University

2015
ABSTRACT

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Abstract

The dipole-flow test is an aquifer characterization technique that utilizes a single-borehole measurement system to yield the vertical hydraulic conductivity, horizontal hydraulic conductivity, and storativity within confined aquifers. The test implements a packer and a pump system that creates a hydraulic dipole flow pattern by pumping water at a constant rate through a suction screen, transferring it within the well to a second chamber, and injecting it back into the aquifer. Various mathematical models have been developed to derive the drawdown in each chamber and estimate water flow parameters. This thesis re-derives and generalizes a new mathematical model for the dipole flow test with asymmetrical chamber lengths.

We also carefully develop a parameter estimation technique for the dipole-flow test. This system consists of two stages: graphical, in which initial estimates of the parameters are fine-tuned, and numerical, which is based on the Newton-Raphson algorithm. This parameter estimation procedure is tested on a synthetic (hypothetical) data set. The results obtained from this computation demonstrated that this developed hydrological model yields accurate parameter estimates from measurements of drawdowns. We conclude that our model provides experimenters with a valuable and efficient mathematical tool for aquifer characterization.
Dedication

I dedicate this thesis to my mother for all her support and encouragement. I appreciate her sacrifices and wouldn’t have been able to pursue my education without her unconditional encouragement and love.
Acknowledgment

I would like to acknowledge Dr. Zbigniew Kabala, my advisor at Duke University. He suggested the thesis topic and pointed me in the most fruitful direction in my literature search. I also learned the basics of Mathematica, which I implemented in this thesis, in his Applied Math for Engineer graduate course. Dr. Kabala guided me patiently and cheerfully through the re-derivation and generalization of his dipole flow test model. He taught me how to use his codes, both in his graphical estimation methodology as well as in his computational approach. By re-analyzing Dr. Kabala’s synthetic examples, I mastered my understanding of data interpretation. This computational environment, capable of symbolic and numerical calculations, will serve me well in my professional life.
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1. Introduction

The current surge in population growth and urbanization has been accompanied with the increasing use of artificial chemicals, the depletion of earth's finite resources, and contamination of previously pristine natural environments. Clean water demand has been rising steadily as the undeveloped world transitions from rural into industrialized and highly consumer-driven societies. This is especially true of regions nearby urbanized city centers and their surrounding suburbs. The extensive use of pesticides, pharmaceuticals, heavy metals, and fertilizers throughout everyday activities make these chemicals abundant at regional scales. Inevitably, they make their way into the nearby streams and watersheds that ultimately feed groundwater reservoirs. Moreover, irregularities in the frequencies of droughts and extreme flood events make water availability unpredictable and, at times, dangerously scarce.

1.1 Groundwater Usage and Contamination

Groundwater poses a particular interest within potable water resources and engineering because of its widespread and abundant use. It is estimated that 36% of earth's population depends solely on groundwater for its drinking supply (45% within the US) (Geological Survey 2008). Similarly, 65% of all agricultural crops are supplied via groundwater sources. However, crucial to human development, groundwater remains a vastly unexplored and underrepresented source (Hutson et al., 2004). Nearby
90% of our freshwater supplies lie underground, but less than 27% of the water Americans use comes from underground sources, which illustrates their underutilization of groundwater (Geological Survey, 2008). According to the National Geographic Society, hydrologists estimate that American groundwater reserves contain at least 33,000 trillion gallons (Hutson et al., 2004). These underground reserves, mostly found within aquifer formations, are challenging to characterize and study due to their inaccessibility. While vital for further development and growth, confined groundwater structures are being polluted at unprecedented rates. This contamination is most prevalent at and around waste disposal sites, industrial facilities, and heavily residential districts. Nitrates, hydrocarbon, and volatile organic compounds together make up the bulk of this chemical contagion, most of which reaches the aquifer through stormwater runoff. Human exposure to these contaminated waters is associated with serious detrimental health effects. Again, affected areas are hard to treat specifically due to the costly, slow, and inefficient technologies available for groundwater modeling and manipulation. Specifically, aquifer characterization is essential for managing and promoting both the extraction of clean groundwater reserves and the remediation of contaminated reservoirs (Colten, 1989).

1.2 Introduction to Aquifers Geomorphology
An aquifer is a geological formation from which groundwater can be extracted using a well. It typically encompasses the body of saturated rock through which the water moves. These structures must be both permeable and porous, and includes a wide variety of rock types such as sandstone, limestone, sand and gravel. The water within the aquifer moves slowly through the porous spaces of the rock, which are too small to sustain life beyond bacteria or viruses. These spaces act as filters for natural purification by removing particulate matter from the liquid as it squeezes through the porous media. Aquifers may occur at various depths, those closer to the surface are not only more likely to be used for water supply and irrigation, but are also more probable to be replenished by the rainfall. Similarly, they are more likely to get contaminated from nearby sources of pollution (Walton, 2007).

Aquifers can either be saturated or unsaturated. A saturated zone or aquifer means that the pore space lies under the water table and is completely filled up (the pressure head of the water is greater than the atmospheric pressure). The unsaturated zone is the portion of the subsurface above the groundwater table. The soil and rock in this zone contains air as well as water in its pores, and cannot be utilized as a source of clean water for human consumption. Aquifers can also be confined or unconfined. Unconfined aquifers are those into which water seeps from the ground surface directly above. Confined aquifers contain an impermeable rock layer that prevents this water recharge. Instead, water enters confine aquifers from farther away where the imperme-
able layer does not exist (Walton, 2007). Hydrologists and water conservationists usually deal with anisotropic aquifer flow (as opposed to isotropic). In isotropic aquifers the hydraulic conductivity is equal for flow in all directions, while in anisotropic conditions it differs (notably between the vertical and horizontal directions) (Stevanovic & Springer, 2015). The hydraulic conductivity (K) refers to the aquifer's ability to transport water through the pore spaces. It is dependent on the permeability of the rock, density and viscosity of the fluid, degree of saturation, and geology of the rock bed (Maliva et al., 2015). The anisotropy ratio (a) relates these hydraulic conductivities in different directions, most notably the horizontal-to-vertical relation (Kr/Kz). The anisotropy ratio is a key factor affecting both water flow and the sizes of capture zones around the vertical-circulation wells.

1.3 Introduction to Aquifer Pumping Tests

The realities of this era bring about new challenges in managing groundwater reserves, including ways to remediate contaminated water for future use and safe release into the environment. The handling of these treatments requires accurate, reliable, and practical models of groundwater flow and contamination transport (Kabala, 1993). The validity of these models relies heavily on the obtainment of specific medium parameters which govern the geophysical processes within the systems. In order to gather this data
scientist turn to various methods of aquifer characterization techniques. Aquifers are characterized in order to shed light into the specific parameters that govern water and contaminant movement within the system. These are crucial in order to continue scientific advancement of treatment technologies, groundwater extraction systems, and ecological preservation regulations.

Aquifers are especially difficult to study because of their constraining environment, frail infrastructure, and scarcity. A series of pumping tests have been devised specifically to evaluate these problematic infrastructures. These tests are generally conducted by stimulating the aquifer through constant pumping and later observing its response via observation wells. "When water is pumped from the pumping well the pressure in the aquifer that contains the well declines. This decline in pressure will show up as drawdown (change in hydraulic head) in an observation well" (Ferris et al., 1962). Drawdown decreases with radial distance from the pumping well and increases with the rate of the pumping. These tests are later interpreted by utilizing analytical models for water flow and matching them to the data observed in the experiment, assuming that the parameters from the idealized model apply to the real-world aquifer (Stevanovic & Springler, 2015).

The three most prevalent tests include slug testing, standard pumping tests, and constant-head tests. These methods differ according to the type of controlled hydraulic stress that the control well imposes on the aquifer system. Their objective is always to
characterize a system of aquifers, as well as to quantify their most relevant parameters: horizontal hydraulic conductivity, specific storativity, and flow velocity (Ferris, 1962). Despite the abundance of field techniques available for aquifer characterization, only a few approaches have been developed and implemented for the determination of the anisotropy ratio between horizontal and vertical conductivities (Hvilshoj & Madsen, 2000). The lack of information on this distribution is currently halting the advancement in groundwater modeling and remediation techniques. Laboratory analyses based on parameter measurements are oftentimes faulty, and yield values that are characteristic of disturbed samples, as opposed to the "undisturbed" aquifers that we find in nature and are trying to parameterize (Hvilshoj & Madsen, 2000). Several methods have been proposed for determining the anisotropy ratio based on pumping wells of partially penetrating wells, however they are extremely costly and time-consuming (Hantush, 1964). Furthermore, the scale of such measurements may not be appropriate for field-scale numerical modeling.

Kabala (1993) was the first to propose yet another pumping test based on the recirculation wells technologies: the dipole flow test. This test can successfully yield both the horizontal and vertical hydraulic conductivities as well as the specific storage coefficient within confined aquifers. This method utilizes vertical recirculation wells in order to acquire hydrologic measurements and compute characteristic parameters. These circulation wells are an in-situ groundwater treatment technology where water is
pumped from one interval in a well, treated within the well bore, and released into another screen into the aquifer. This movement of pressurized water, caused by the constant water source and sink wells, could be utilized to obtain the hydraulic head resulting from multiple line sinks and sources in homogeneous confined aquifers. In turn, these heads can then be mathematically manipulated to calculate the hydraulic head gradient and velocity fields (Zlotnik & Ledder, 1996). Both of these parameters are needed in modeling contamination flow and help yield values for aquifer parametrization. Though still novel and widely unexplored, recirculation wells and the theory of the dipole flow hold noteworthy implication for the development of cost efficient, timely, and effective water remediation/ aquifer characterization solutions.

1.4 Introduction to Recirculation Wells and Tests

Vertical groundwater recirculation wells were developed and utilized to treat contaminated water and soil. The primary advantage of this technique is that its in situ implementation allows aquifers to be treated without bringing the polluted water up into the surface, thus also eliminating the need to dispose of the hazardous waste. Another benefit is that it works while creating a very low disturbance of the water table, which is ideal when treating delicate environments such as marshes and swamps (Herrling et al. 1991). Vertical wells are primarily utilized when dealing with persistent hydrocarbons
and other persistent substances. Furthermore, they are relatively low-cost and require a short time period for installation and implementation, which makes them ideal for state water management districts.

The vertical recirculation well apparatus is primarily exploited for the study and characterization of water reservoirs. One significant application to the study of recirculation wells models is that these form the bases of a proposed method for determining aquifer parameters from analysis of transient pressure head drawdown (Kabala, 1993). It is widely thought that simple-borehole tests, including the dipole flow tests, are the most economically friendly and easiest technologies for aquifer characterization. The tests typically also simulate water flow and velocities, which are critical in determining how quickly contaminants will dissipate and reach catchment, rivers, and ponds. These findings, in turn, allow public and private entities to determine the appropriate aquifer water supply, risk management and remediation techniques. The test is oftentimes also used to remove contaminants within the well, thus making groundwater fit for human consumption and retention. This well is an in situ technology, which allows for the treatment of water without having to extract it from the contaminated medium. The wells consists of two screened sections (chambers) separated by an impermeable casing. One chamber, the inlet screen, absorbs aquifer water while the other section (outlet screen) injects it back out into this same aquifer (Kabala, 1993). The water is drawn into the well through the inlet screen and then treated by one of several processes before its
final exit out of the device. This clean water is released through the outlet screen and reintroduced back into the aquifer, preventing a net withdrawal of water. The displaced water is generally driven by a system of pumps that promote movement due to gravity and other applied pressures (Schaad, 1998).

Figure 1- Demonstration of packer to be introduced below the groundwater table and into the aquifer (Schaad, 1998).

Figure 2- Close-Up of the upper chamber within the packer (Schaad, 1998).

Discharged water flows under the influence of vertical gradients created during the extraction process at the inlet screen and the compression at the outlet screen. This
process creates a recirculation zone that typically returns the majority of the treated water back into the inlet screen. Therefore, the water cycles back through the entirety of the treatment system several times before escaping from the well. This occurrence makes the treatment highly efficient: the water does not have to achieve final cleanup levels in the first pass since it will return for additional treatment. The shape and size of the area of influence and treatment zone are largely determined by the hydraulic conductivities, pumping rate, radius of the well, and anisotropy of the aquifer (Sutton et al., 2000). Similarly, characteristics of major interest in aquifer remediation also include the head differences between the chambers as a function of pump flow rate, aquifer sorption and well parameters (Zlotnik, 1998).

1.5 Introduction to the Dipole Flow Test

A dipole flow is the hydrological flow induced by the vertical circulation well containing both the injection and extraction chambers within a single borehole. This movement arises out of the superposition of a sink and source of equal intensity placed symmetrically with respect to the same origin (Kabala & El-Sayegh, 2002). The dipole flow follows the same physical principles of electricity and magnetism. For instance, within the classical realm of electromagnetism, an electric dipole is created by charged objects with equal but opposite electric charges that are separated by a distance. The
dipole moment is a measure of the positive and negative electric charges within the medium, and exhibits a pattern of force fields which are nearly identical to the ones that are created within the hydraulic dipole flow tests (Kholmetskii et al., 2013).

The hydrologic dipole flow test evolved as a means of utilizing this model of recirculation flow to evaluate and predict aquifer properties (Kabala, 1993). During the test, water is pumped at a constant rate $Q$ across the entirety of the system; meanwhile data (such as pressure gradients) are gathered for investigation. This investigation involves the interpretation of the head in the two chambers, which are isolated from each other by a multipacker system (Johnson & Simon, 2007). Specifically, this test is effective in determining the vertical distributions of both the horizontal and vertical hydraulic conductivity, as well as the specific storativity. This is significant because hydraulic conductivity is arguably the most relevant measure for assessment of contami-
nation transport, precisely because it governs the rate at which the fluid moves through
the porous rock media (Roose, 2009). Also, the dipole-flow test allows one to accurately
estimate the effective hydraulic conductivity anisotropy ratio \((K_r/K_z)\), which is crucial
for determining the size of the capture zone of the vertical-circulation well and thus the
spacing between such wells.

The construction and implementation of the dipole flow device is fairly simple
and economic. A submersible pump located at the center of the packer assembly drives
water movement through the device. The packer length is determined by the geology of
the terrain, proposed pumping rate, and specific experimental objectives. Pressure
transducers are mounted in the packers and connected to the chambers in order to moni-
tor pressure changes, as well as to guard against leaks. A pump controller and electric
generator are connected to the apparatus and maintained above ground for periodic
checkups. Once that steady state-condition has been reached, a reactive tracer could be
injected into the stream and monitored to create breakthrough curves. These generated
curves can be further evaluated at the lab with simulation modeling for aquifer characteri-
ization. For instance, the chamber pressure changes could be matched to type curves
generated from an analytical solution to estimate aquifer parameters (Sutton et al.,
2000).
Figure 4- Prototypical dipole flow technology (modified from Zubuchen, 2010).

The dipole flow test offers many advantages over the other traditional pumping tests. For example, it requires a very short experimental time and a more simplified data performance interpretation. The dipole flow test also eliminates the need for water disposal, and provides instantaneous signals of possible hardware failures while testing. Unlike most other in situ treatments, it minimizes site disturbance and provides real-time assessments of the data collected. The dipole flow effects created by the well decreases rapidly with distance, so that far from the cylinder we find an undisturbed flow (Zlotnik et al., 2007). The test was first implemented for parameter estimation at the Lizzie field site in North Carolina as part of a doctoral dissertation from Duke University (Schaad, 1998). Thereafter, numerous other field studies were conducted with varying diameter wells, dipole configurations, and flow rates. The hydraulic conduc-
tivity profiles generated by these tests closely resemble the values and trends estimated through pump tests, sieve analysis, and flowmeters (Roose, 2009). The potential problem with recirculation tests is the short-circuiting of flow through the disturbed zone or well skin. Since these tests induce a predominantly vertical flow field, the well skin may be more pronounced in the flow than in other single-borehole tests (Kabala, 1993; Zlotnik et al., 1998). However, this short-circuiting through the skin is not a problem in dipole flow tests conducted on the vertical circulation wells, as these have the skin between the chambers screens sealed with bentonite (Johnson & Simon, 2007).
2. Objective

This thesis attempts to lessen the challenges presented within aquifer characterization by furthering our development of the dipole flow tests and its many applications. In this document we present a novel mathematical model for determining the drawdowns, draw-ups, and related parameters for confined, homogenous, and anisotropic aquifers. We aim to develop a model that yields more accurate values which would better estimate those observed in the field and captured by sensors. In order to do so we re-derive and generalize the existing dipole flow model presented by Kabala in 1993. Specifically, we allow for asymmetrical chamber sizes and account from transient response.

Based on this model we then develop a two-stage parameter estimation technique: graphical and numerical. In the graphical stage we develop an initial investigational guess for the three crucial aquifer parameters (Kr, Kz, Ss) which produce a response similar to the one measured on the field tests. In the numerical stage we later use the Newton-Raphson algorithm to refine our initial values for the three parameters. Contrary to the claims of Hvilshoj et al. (2000), we intend to demonstrate that a parameter estimation procedure based on the Newton-Raphson algorithm, which leads to least-square parameter estimates, is actually robust.

The tertiary objective is to test the parameter estimation technique on a synthetic/ hypo-
theoretical example and to demonstrate its robustness. It will also serve as a guide prototype for future recreating of the formulas. The last objective of this research was, if time permits, to analyze some of the unanalyzed data from the Johnson and Simon 2007 paper.
3. Literature Review

The endeavor to estimate the hydraulic properties of aquifers first arose from the need to explore their potential for supplying water. The worth of an aquifer as a fully developed source of water initially depends largely on two inherent characteristics: its ability to store and its ability to transmit water (Ferris et al., 1962). For decades the main objective of groundwater science within the U.S Geological Survey was to evaluate the availability, quality, and ease of extraction from viable sources. The lack of technology created circumstances which required tests to be conducted without prior knowledge of the geology within the vicinity of the site. This uncertainty reduced the reliability of the test results to a "semiquantitative category" (Ferris et al., 1962). Additionally, over the past few decades, scientists have become increasingly interested in aquifer flow due to the heightened concern in environmental contamination problems. The resolution of these problems requires that hydraulic characterization be carried out at a much finer spatial scale for which adequate information is presently scarce.

3.1 Fundamentals of Groundwater Hydrology

The first reported studies carried out to understand the flow of water through capillary tubes were conducted by Hagen and Poiseuille in the early 1840s. Developments in fluid mechanics, such as the Darcy equations and Muskat theories, soon
advanced the understanding of the transient flow process and enabled further development of testing mechanisms. In 1863, Dupuit applied Darcy's law to well hydraulics, using an ideal case of a well located at the center of a circular island (Bruin & Hudson, 1961). Over half a decade later, the transient diffusion equation proposed by Fourier became the basis for inverting hydraulic tests data to estimate two basic parameters: hydraulic conductivity and hydraulic capacitance (Narasimhan, 1998).

### 3.2 History of Aquifer Testing

The first successful test on record within the Water Resource Journals filed by water survey personnel was conducted on a municipal well at Lawrenceville, IL, in 1922 (Bruin & Hudson, 1961). A number of years later, the first successful attempt to analyze the nonsteady flow to a penetrating well in an unconfined aquifer, while maintaining a constant drawdown, was carried out by Weber in 1928. The idea of a coefficient of permeability (P), which is a measure of a materials' ability to transfer water, and is related to hydraulic conductivity, was first expressed by Meinzer in 1928. A huge milestone in the science of aquifer characterization came about in 1935 by Theis' development of a mathematical model for the nonsteady flow of ground water. He derived the nonequilibrium formula "from the analogy between the hydraulic conditions in an aquifer and the thermal conditions in an equivalent thermal system" (Ferris et al., 1962).
This same year Theis also introduced the concept of a transmissivity coefficient
(T=K*b), which is the rate of flow under a unit hydraulic gradient through a unit width
within an aquifer of a given saturated thickness. This finally enabled hydrologists to
predict the recovery and future changes in groundwater drawdowns resulting from
pumping or recharging wells (Bruin & Hudson, 1961).

In the 1930s, these successes led to a systematic analysis of pressure transients from
aquifers and petroleum reservoirs. Jacob further verified the derivation of the nonequilib-
rium formula directly from hydraulic concepts in 1940. This formula in nondimensional
form would then take its popular form as:

\[ s = \frac{Q}{4\pi T} \int_0^\infty \frac{e^{-y}}{y} dy \]

where (Ferris et al., 1962). This simple equation is the one that sets the stage and forms
the foundation for our hydrologic analysis and development of a new model.

### 3.2.1 Aquifer Pump Testing in the 1950s

As field experience increased, confidence in the applicability of quantitative
methods was gained, which in turn stimulated the interest in developing solutions for
more complex hydrologic problems. In his 1940 paper, Hubbert derived a tangent law
for the refraction of flow lines, and went on to establish the foundations for the study of
regional groundwater systems and petroleum reservoirs. A decade later, Jacob promoted
the use of a storage coefficient \( S = S_s \times b \), which is defined as the volume of water that it releases from or absorbed into the aquifer storage per unit surface area given the unit head change (Ferris et al., 1962). Skempton (1954) contributed broadly to the topic of soil - water mechanics by proposing pore pressure coefficients which quantified the relationship between external stress changes and the changes in pore fluid pressure within saturated soils (Narasimhan, 1998). Similarly, Skibitzke (1958) developed a technique for determining the transmissibility coefficient from the recovery of the water level in a well that had been previously drained. That very same year, Jacob and Lohman derived a formula for determining the storage and transmissivity coefficients from a test in which the discharge varied with time while maintaining a constant drawdown (Narasimhan, 1998). Along with all of these advancements, the very first definitive textbook on groundwater hydrology was finally published by Todd in 1959. It talked in extensive detail about hydraulics and presented a comprehensive literature on the topic (Ferris et al, 1962).

3.2.2 Aquifer Pump Testing and Modern Technology

The creation of the digital computer revolutionized the science of groundwater hydrology in the 1960s. This technology afforded the possibility of solving transient fluid problems in complex geological systems which had previously been too multi-
faceted for closed-form solutions (Narasimhan, 1998). With the help of fast processing computers, the finite element methods, which had been initially designed for structural engineering problems, was soon enhanced to solve transient problems of groundwater flow (Javandel & Witherspoon, 1968). Similarly, Fayers and Sheldon (1962) transformed the field of petroleum engineering by solving fluid flow problems in three dimensions using classical finite difference approximations via computer software. In the field of civil engineering, Tyson and Weber (1964) presented an integral form of the finite difference method which could efficiently handle groundwater systems with complex geometries (Narasimhan, 1998). Vertical recirculation wells did not develop until the 1960s. Though the necessary technologies and geographical formations for this experiment had been in place for years, the science of modeling and hydrologic analyses lagged behind most of the other pumping tests (Ferris et al., 1962). The 1970s witnessed a shift in research emphasis among earth scientists from issues based on resource attainment to the topics of environmental degradation. In 1972, Neuman devised a means of utilizing the vertical anisotropy to account for the pressure transient behavior of unconfined aquifers. Efforts were also made to understand and model flow within the vadose zone. Weeks (1978) developed a field method for evaluating pneumatic conductivity and diffusivity in this zone "based on transmission of barometric pressure changes from the land surface to the water table" (Narasimhan, 1998).

The focus of groundwater management underwent yet another transition through-
out the 1980 s. Groundwater contamination arising from leaky gasoline tanks and pollution arising from the uncontrolled disposal of industrial hydrocarbons became the emphasis of hydrologic science. Advancements in soil physics also made it possible to apply already established theoretical results to devise instruments to estimate hydraulic characteristics of unsaturated soils in the field. Additionally, measuring the vertical hydraulic conductivities of the soil surfaces was made possible by the creation of the disc tension. This instrument works by applying a constant moisture tension boundary condition at the land surface to enable infiltration at lowered water potentials. Many breakthroughs to come benefitted from, and were made possible by, this and other similar field instruments (Narasimhan, 1998). Herrling and Stamm (1992) were some of the first to investigate the general features of vertically circulating flow fields in support of their use as a remedial technology. They estimated a flow field from a "three-dimensional numerical model simulating a radially symmetrical flow in a confined aquifer" (Mohamed et al., 2006). This approach was later used to generate a host of relationships to aid the design of various remedial systems. That very same year another analytical model was developed for simulating the flow field and fluid path lines in a homogeneous, anisotropic, confined aquifer with a regional gradient (Philip & Walter, 1992). "They used the hydraulic head change due to a point sink in an infinite porous medium, the principle of superposition to develop a line sink/source, the method of images to satisfy the confined aquifer boundary conditions, and spatial scaling to account for the effects of an
anisotropic hydraulic conductivity field" (Mohamed et al., 2006). This tool was implemented in determining optimal designs for well configurations and well screen dimensions.

3.3 Development of the Dipole Flow Test

Thus far, most traditional methods of analysis of field parameters have relied heavily on analytic solutions to specific and highly idealized problems. New methods, such as the dipole flow test attempts to breech the gap between idealized systems and actual values. This test utilizes the basic vertical recirculation test previously explained and various hydrologic principles to obtain precise vertical and hydraulic conductivities. This test shows promise in overcoming the huge time, expense, complexity, and water disposal requirements currently necessary to characterize contaminated aquifers. Before this there were no analytical solutions of the drawdown and flow field induced by a circulation well. Previously these results were obtained through computer-intensive modeling simulations, "including detailed finite and boundary element modeling and particle tracking methods" (Zlotnik & Ledder, 1996). Similarly, all past literature had solely measured the horizontal hydraulic conductivity and neglected the vertical hydraulic conductivity along with its many applications, which are crucial for three-dimensional modeling of contaminant fate and for determining the spacing of vertical-circulation wells for aquifer remediation. Knowledge of this parameter is necessary in
order to implement many newly developed circulation remediation procedures. The test achieved results from its model of mathematical implementations of the superposition principles, and allowed for the direct calculation of path lines in a dipole flow field. This mathematical model assumes that the experiment is conducted within a fully penetrating well which is homogeneous, radially symmetric, confined, and of finite extent. Kabala’s publications also dealt exclusively with simplified scenarios void of the skin effect, well losses, and well bore storages. Zlotnik and Ledder (1994) extended the findings to develop similar mathematical models with a focus in understanding the kinematic flow structure around the device and the drawdown in the well chambers in a uniform, anisotropic, infinite aquifer. Specifically, they utilized a Taylor series expansion of the solution of the total drawdown to investigate the region of influence by treating the injection/extraction chambers as either a point or linear sink/sources.

Dr. Kabala and his graduate student, David Schaad, at Duke University where the first researchers to construct, utilize, and measure the dipole flow test (1998). Later, Zlotnik and Zurbuchen (1998) refined "construction details of a dipole system and related components, and provided guidelines for the interpretation of pseudo steady-state flow" (Mohamed et al., 2006). Halihan and Zlotnik (2002) developed a steady-state model for asymmetric dipole-flow test, i.e., one with different sizes of the chambers. Their formulation allows for estimation of horizontal hydraulic conductivity given knowledge of the hydraulic conductivity ratio. Halihan also thoroughly described the
"applicability of the continuum and discrete approaches for the conceptualization of groundwater flow" (Halihan & Zlotnik, 2002). Because the head changes in the chambers were of unequal length, the tests used two different hydraulic signals during the same test to evaluate aquifer geometry (Halihan & Zlotnik, 2002). Since this knowledge is unavailable, the authors apply their solutions under the assumption that the aquifer is isotropic, i.e., its anisotropy ratio $K_r/K_z = 1$. In contrast to Halihan and Zlotnik (2002), we develop here a transient model for asymmetric dipole-flow test that allows estimation not only of horizontal hydraulic conductivity, but also that the anisotropy ratio, $K_r/K_z$, and specific storativity, $S_s$. There have also been substantial advancements in the understanding and modeling of the dipole flow geometries, regardless of their medium. The dispersion process within this flow seems to be characterized by a power-law decay of tracer concentrations with respect to time, with an experimental cutoff at very long times (Kurowski et al., 1994). Many tests have shown that transmission tracer dispersion in a dipole geometry exhibits characteristics that are completely different from those of a traditional Gaussian tracer dispersion in flows of porous media (Kholmetskii et al., 2013).

Physical dipole flow tests can be conducted in a single vertical configuration well (Kabala 1993; Zlotnik & Ledder 1996; Zlotnik & Zurbuchen 1998), in multiple wells to conduct horizontal tests (Clement et al.1997), or combining both approaches (Hvilshoj et al.2000). The dipole flow test has already been executed and extensively
field tested within the Management System Evaluation Areas in Nebraska (Zlotnik & Zurbuchen 1998), the Clare Valley, South Australia (Halihan, 2000), the GEMS site in Kansas, USA (Zurbuchen et al.1998), the Vejen site, Denmark (Hvilshoj et al.2000), and the Horkheimer Insel site, Germany (Zlotnik et al.2001). In 2007, the dipole flow test was applied to investigate the effects of entrapped air on saturated hydraulic conductivity in a cylindrical aquifer model (Zlotnik et al., 2007). The drawdown within the medium was found to be linear to the flow rate with exception of the areas immediately outside the dipole chambers. Following this publication, Hvilshoj conducted an analysis with the intent of testing different interpretation methods. Hvilshoj et al.(2000) concluded that the analytical solutions for the dipole flow test in conjunction with Newton - Raphson algorithm or nonlinear regression optimization "did not lead to acceptable results." We disagree. We contend that Hvilshoj et al. (2000) field tests suffered from skin effect and had too small response time scale to be meaningfully analyzed. One of the goals of this thesis is to demonstrate that the Newton - Raphson parameter estimation procedure, which leads to least - square parameter estimates, is actually robust for the interpretation of the dipole flow test data.
Chapter 4: Re-development and Generalization of the Dipole-Flow Test Model

4.1 Dipole-Flow Test: the idea and its limitations

As mentioned earlier, Kabala [1993] proposed the dipole-flow test for aquifer characterization that does not induce large drawdowns and does not bring, possibly contaminated groundwater, to the surface. The presented solution was developed in terms of the Fourier series for aquifers of arbitrary extent. Zlotnik and Lederer [1996] studied the test for a case of aquifers of infinite extent. Zlotnik and co-workers focus on the steady-state test and miss thus its potential for estimating hydraulic conductivity anisotropy ratio, $\frac{K_y}{K_z}$, and specific storativity, $S_s$. Kabala [1993] and Zlotnik and Lederer [1996] studied the dipole flow test for the case of upper and lower chamber of equal sizes. However, for various reasons, the vertical-circulation wells used for aquifer remediation are constructed often with chambers of different sizes (e.g., Johnson and Simon, 2007). Although Halihan and Zlotnik (2002) developed a steady-state model for asymmetric dipole-flow test, i.e., one with different chamber sizes, they focus, as does Zlotnik and his other co-workers, on the steady-state test (usually under the assumption of aquifer hydraulic isotropy) and miss thus the potential of the test for estimating aquifer hydraulic conductivity anisotropy ratio, $\frac{K_y}{K_z}$, and specific storativity, $S_s$. For this reason, we re-develop here the mathematical model of the dipole flow test for the gen-
eral case when these chambers are of arbitrary sizes and the test response is transient. We note that when applied down a regular borehole, the dipole-flow test typically suffers from the short-circuiting flows through the skin around the well. However, with usually perfect bentonite seal of the gravel envelope between the chambers, vertical-circulation wells built for aquifer remediation are ideally suited for conducting the dipole-flow test for aquifer characterization. These tests do not suffer from the skin effect.


Consider the schematic of the dipole-flow test.
This schematic differs from that of Kabala’s (1993) by allowing for different lengths of the upper chamber, $\Delta_u$, and the lower chamber, $\Delta_L$. With this modification, we follow here closely the derivation of Kabala (1993). The length parameters $r_w$, $b$, $l$, $d$, and $\Delta_L$ are defined in that schematic.

We use in the process the formulas developed by Hantush (1964) for average drawdown in an observation well (designated # 4) and induced by pumping of a partially penetrating well (designated # 3), as seen in the schematic from Hantush (1964, p. 348, Fig. 10).

The length parameters $r$, $b$, $l$, $d$, $d'$, and $l'$ are clearly defined in that schematic:
The Hantush solution for average drawdown in an observation well in an anisotropic aquifer follows from Hantush (1964, eqns 73 and 74, p. 350) by averaging the \( \cos(n \pi z/b) \) term for \( d' < z < l' \), which was published by Hantush (1961, eqns 9a and 9b, p. 90). The solution is

\[
S(t) = \frac{Q}{4 \pi K_r b} \left\{ W(u_r, \beta_w) + \frac{2 b^2}{\pi^2 (1 - d) (l' - d')} \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin \left( n \pi \frac{1}{b} \right) - \sin \left( n \pi \frac{1 - d}{b} \right) \right] \right\}
\]

where, with \( L \) denoting a length unit and \( T \) a time unit, \( S(L) \) is the drawdown in the upper chamber, \( t(T) \) is time from the beginning of pumping, \( W(u, \beta) \) is the *leaky aquifer function* of Hantush (1961, 1964)

\[
W(u, \beta) = \int_{u}^{\infty} \frac{e^{-\frac{\sqrt{y}}{\sqrt{\beta}}}}{\sqrt{y}} \, dy
\]
and

\[ \nu_r = \frac{K_r}{S_s} \quad \quad u_r = \frac{r_w^2}{4 \nu_r \tau} \quad \quad a^2 = \frac{K_r}{K_z} \]

(3)

\[ B_r^2 = \frac{K_r b}{K' / b'} \quad \quad \beta_w = \frac{r_w}{B_r} \]

where \( Q \left( L^3 / T \right) \) is the pumping rate (\( Q > 0 \) for pumping or removing water and \( Q < 0 \) for injecting water); \( K_r \) and \( K_z \) (L/T) are hydraulic conductivities in r an z directions, respectively; \( K' \) is the hydraulic conductivity (L/T) of the leaky layer; \( S_s \) is specific storativity for confined aquifers or specific yield for unconfined aquifers (1/L); \( \nu_r \) is the hydraulic diffusivity \( (L^2 / T) \); \( a^2 \) is the hydraulic conductivity anisotropy ratio (dimensionless); \( u_r \) is the dimensionless inverse of time; and \( \beta_w \) is the dimensionless leakage factor. The other length parameters such as \( l, d, \Delta_u, \Delta_L, b, b', r, \) and \( r_w \) are defined in the figures above.

**NOTE:** In what follows we assume that the upper chamber is pumped (Q) while the lower chamber is injected (-Q). If the opposite is true, all one needs to do in the formula derived below is to replace Q with -Q.

### 4.2.1 The Upper-Chamber Drawdown

The drawdown in the upper chamber due to pumping water with volumetric flow rate \( Q \) from that chamber follows from (1)--the partially screened observation well is here identical with the upper chamber and so is the partially penetrating well:
An analogous expression for the drawdown (drawup) in the upper chamber due to the injection of the lower chamber with volumetric rate \(-Q\) is:

\[
 s(t) = \frac{Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{b^2}{2\pi^2 \Delta_u^2} \right\} + \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin \left( n\pi \frac{d + 2\Delta_u}{b} \right) - \sin \left( n\pi \frac{d}{b} \right) \right]^2 W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{a b} \right)^2} \right)
\]

According to the trigonometric identity \# 1 derived in Appendix B, we have

\[
 \sin \left( n\pi \frac{d + 2\Delta_u}{b} \right) - \sin \left( n\pi \frac{d}{b} \right) = 2 \sin \left( n\pi \frac{\Delta_u}{b} \right) \cos \left( n\pi \frac{d + \Delta_u}{b} \right)
\]

and

\[
 \sin \left( n\pi \frac{1}{b} \right) - \sin \left( n\pi \frac{1 - 2\Delta_L}{b} \right) = 2 \sin \left( n\pi \frac{\Delta_L}{b} \right) \cos \left( n\pi \frac{1 - \Delta_L}{b} \right)
\]

With these identities, equations (4) and (5) reduce themselves to

\[
 s(t) = \frac{Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{b^2}{2\pi^2 \Delta_u^2} \right\} + \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ 2 \sin \left( n\pi \frac{\Delta_u}{b} \right) \cos \left( n\pi \frac{d + \Delta_u}{b} \right) \right]^2 W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{a b} \right)^2} \right)
\]
s(t) = \frac{-Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{b^2}{2\pi^2 \Delta_L \Delta_u} \right\} \left[ \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ 2 \sin \left( n \pi \frac{\Delta_L}{b} \right) \cos \left( n \pi \frac{1 - \Delta_L}{b} \right) \right] \right]

\left[ 2 \sin \left( n \pi \frac{\Delta_u}{b} \right) \cos \left( n \pi \frac{d + \Delta_u}{b} \right) \right] \sqrt{W(u_r, \sqrt{\beta_w^2 + \left( \frac{n \pi r_w}{a b} \right)^2}}

Finally, since the governing partial differential equation for drawdown in the aquifer is linear, we can employ the superposition of solutions (6) and (7) and arrive at the upper-chamber drawdown as

s(t) = \frac{Q}{2\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin \left( n \pi \frac{\Delta_u}{b} \right)}{n \pi \frac{\Delta_u}{b}} \right]^2 \left[ \frac{\cos \left( n \pi \frac{d + \Delta_u}{b} \right)}{n \pi \frac{\Delta_u}{b}} \right]^2 - \frac{\sin \left( n \pi \frac{\Delta_L}{b} \right)}{n \pi \frac{\Delta_L}{b}} \frac{\sin \left( n \pi \frac{\Delta_u}{b} \right)}{n \pi \frac{\Delta_u}{b}} \cos \left( n \pi \frac{1 - \Delta_L}{b} \right) \cos \left( n \pi \frac{d + \Delta_u}{b} \right) \sqrt{W(u_r, \sqrt{\beta_w^2 + \left( \frac{n \pi r_w}{a b} \right)^2}}

We note that when the sizes of the chambers are the same, i.e., \Delta_u = \Delta_L = \Delta, then (8) reduces to

s(t) = \frac{Q}{2\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin \left( n \pi \frac{\Delta}{b} \right)}{n \pi \frac{\Delta}{b}} \right]^2 \left[ \frac{\cos \left( n \pi \frac{d + \Delta}{b} \right)}{n \pi \frac{\Delta}{b}} \right]^2

\left[ \cos \left( n \pi \frac{d + \Delta}{b} \right) - \cos \left( n \pi \frac{1 - \Delta}{b} \right) \right] \sqrt{W(u_r, \sqrt{\beta_w^2 + \left( \frac{n \pi r_w}{a b} \right)^2}}

With the trigonometric identity # 2 derived in Appendix B, we have the upper chamber
drawdown for $\Delta_U = \Delta_L = \Delta$ as
\[
s(t) = \frac{Q}{\pi K_r b} \left[ \sum_{n=1}^{\infty} \left( \frac{\sin(n \pi \frac{\Delta}{b})}{n \pi \frac{\Delta}{b}} \right)^2 \sin\left( n \pi \frac{d+1}{2 b} \right) \sin\left( n \pi \frac{1-d-2\Delta}{2 b} \right) \right] \cos\left( n \pi \frac{d+\Delta}{b} \right) W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n \pi r_w}{a b} \right)^2} \right)
\] (9)
which is identical with Kabala[1993, eqn 5].

In conclusion, The upper-chamber drawdown in the dipole-flow test is given by eqn (8).

When the sizes of the chambers are the same, i.e., $\Delta_U = \Delta_L = \Delta$, then (8) reduces to (9), i.e., to Kabala[1993, eqn 5].

4.2.2 The Lower-Chamber Drawdown

The drawdown (negative) in the lower chamber due to injecting water with volumetric rate $-Q$ into that chamber follows from (1)--the partially screened observation well is here identical with the lower chamber:
\[
s(t) = \frac{-Q}{4 \pi K_r b} \left( W(u_r, \beta_w) + \frac{b^2}{2 \pi^2 \Delta_L^2} \right) \sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin\left( n \pi \frac{1}{b} \right) - \sin\left( n \pi \frac{1-2\Delta_L}{b} \right) \right]^2 W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n \pi r_w}{a b} \right)^2} \right)
\] (10)
Further following Kabala (1993), we write an analogous expression for the drawdown in the lower chamber due to pumping of the upper chamber with volumetric rate $Q$. Again, it follows from (1)--the partially screened observation well is here identical with the
lower chamber:

\[
s(t) = \frac{Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{b^2}{2\pi^2 \Delta_L \Delta_u} \right\} 
\sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin \left( \frac{n\pi}{b} \right) - \sin \left( \frac{n\pi - 2\Delta_L}{b} \right) \right]
\]

(11)

With the trigonometric identity # 1 from Appendix B employed earlier, (10) and (11) reduce themselves to

\[
s(t) = \frac{-Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{2b^2}{\pi^2 \Delta_L^2} \right\} 
\sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin \left( \frac{n\pi \Delta_L}{b} \right) \cos \left( \frac{n\pi - \Delta_L}{b} \right) \right]^2 W\left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{a b} \right)^2} \right)
\]

(12)

and

\[
s(t) = \frac{Q}{4\pi K_r b} \left\{ W(u_r, \beta_w) + \frac{2b^2}{\pi^2 \Delta_L \Delta_u} \right\} 
\sum_{n=1}^{\infty} \frac{1}{n^2} \left[ \sin \left( \frac{n\pi \Delta_L}{b} \right) \cos \left( \frac{n\pi - \Delta_L}{b} \right) \right] 
\left[ \sin \left( \frac{n\pi \Delta_u}{b} \right) \cos \left( \frac{n\pi + \Delta_u}{b} \right) \right] W\left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{a b} \right)^2} \right)
\]

(13)

Finally, since the governing partial differential equation for drawdown in the aquifer is
linear, we can employ the superposition of solutions (12) and (13) and arrive at the
lower-chamber drawdown as

\[ s(t) = \frac{-Q}{2\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin \left( n \pi \frac{\Delta_u}{b} \right)}{n\pi} \right]^2 \left[ \cos \left( n \pi \frac{1 - \Delta_L}{b} \right) \right]^2 - \frac{\sin \left( n \pi \frac{\Delta_u}{b} \right)}{n\pi} \frac{\sin \left( n \pi \frac{\Delta_w}{b} \right)}{n\pi} \cos \left( n \pi \frac{1 - \Delta_L}{b} \right) \]

\[ \left( n\pi \frac{1 - \Delta_L}{b} \right) \cos \left( n \pi \frac{d + \Delta_u}{b} \right) \right) W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{ab} \right)^2} \right) \]

We note that when the size of the chambers is the same, i.e., \( \Delta_u = \Delta_L = \Delta \), then (14) reduces to

\[ s(t) = \frac{-Q}{2\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin \left( n \pi \frac{\Delta}{b} \right)}{n\pi} \right]^2 \cos \left( n \pi \frac{1 - \Delta}{b} \right) \]

\[ \left( \cos \left( n\pi \frac{1 - \Delta}{b} \right) - \cos \left( n \pi \frac{d + \Delta}{b} \right) \right) W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{ab} \right)^2} \right) \]

or, with the trigonometric identity # 2 derived in Appendix B, to

\[ s(t) = \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin \left( n \pi \frac{\Delta}{b} \right)}{n\pi} \right]^2 \sin \left( n \pi \frac{d + 1}{2b} \right) \sin \left( n \pi \frac{1 - d - 2\Delta}{2b} \right) \]

\[ \cos \left( n \pi \frac{1 - \Delta}{b} \right) W \left( u_r, \sqrt{\beta_w^2 + \left( \frac{n\pi r_w}{ab} \right)^2} \right) \]

(15)

which is identical with Kabala [1993, eqn 6].

In conclusion, the lower-chamber drawup in the dipole-flow test is given by eqn (14).

When the size of the chambers is the same, i.e., \( \Delta_u = \Delta_L = \Delta \), then it reduces to (15),
which, again, is identical with Kabala [1993, eqn 6].

### 4.3 Special Functions of Well Hydraulics: $W[u, \beta]$ and its Derivatives

#### 4.3.1 The Hantush (1961) leaky well function, $W[u, \beta]$

The Hantush (1961) leaky well function, $W[u, \beta]$, given by (2) is again

$$W(u, \beta) = \int_u^\infty e^{-\frac{y}{4y} \frac{\beta}{4y}} dy$$

For sufficiently small $u$ values, we have

$$u < \frac{\beta^2}{20} \implies W[u, \beta] \approx 2K_0(\beta)$$

where $K_0$ is the zeroth-order modified Bessel function of the second kind. Since it has no closed-form representation, $W(u, \beta)$ has to be defined as a numerical integral:

- **Definition # 1 for $W(u, \beta)$ via numerical integration:**

  $$W_1[u_-, \beta_] := \text{NIntegrate}\left[\frac{e^{-\frac{y}{4y} \frac{\beta}{4y}}}{y}, \{y, u, \infty\}\right]$$

Alternatively, the function $W(u, \beta)$ can be defined as an inverse Laplace transform that can be inferred from Hantush (1964, p. 303)

$$W(u, \beta) = \mathcal{L}^{-1}\left\{\frac{2}{p} K_0\left(\sqrt{p + \beta^2}\right), p \rightarrow u\right\}$$

- **Definition # 2 for $W(u, \beta)$ via numerical inversion of (14) via the Stehfest (1971) algorithm. Coding of this definition is relegated to the package named Hantush.m.**

**Loading Package Hantush.m with $W(u, \beta)$ defined via a numerical Laplace Inverse Transform via the Stehfest (1971):**
NOTE: to load a Mathematica package, you need to specify the full path to it in your file system.

- In Unix it will be current home director (~) along with the list of directories down to the package file or the full path from the root directory (/.../.../file.m), for example
  - `<< ~/teaching/advising/Michelle_Embon/Hantush.m`
  - `<< /home/kabala/teaching/advising/Michelle_Embon/Hantush.m`
- In Windows it will be similar, but the directories are separated with backward slash rather than the forward slash.

### 4.3.2 Comparison of the two leaky aquifer well functions

\[ W[0.001, 0.1] = 4.82924 \]

\[ W_1[0.001, 0.1] = 4.82924 \]

Let us time the calculation of 10,000 evaluations of function \( W[u, \beta] \) produced 30 times to allow for variations in available computational resources to the operating system, and let us compare these times to their analogues for \( W_1[u, \beta] \).

\[ W\text{times} = W_1\text{times} = \text{Table}[0, \{i, 1, 30\}]; \]
\[ \text{Timing[Do}[W[0.001, 0.1], \{i, 1, 10000\}]] \]
\[ \{1.580000, \text{Null}\} \]
\[ \text{Timing[Do}[W_1[0.001, 0.1], \{i, 1, 10000\}]]\{1\]}
\[ 68.402000 \]
Do[Wtimes[[j]] = Timing[Do[W[.001, 0.1, {i, 1, 10000}]], {j, 1, 30}];
( Do[W1times[[j]] = Timing[Do[W1[.001, 0.1, {i, 1, 10000}]], {j, 1, 30}]; *)
{Total[W1times], Total[Wtimes]}
{2006.1340, 46.0640}

The total calculation time with the two definitions was 2006.13 seconds vs 46.06 seconds.

2006.13 / 46.06
43.5547

Conclusions:
For 30,000 evaluations the function \( W_1(u, \beta) \) took 2,006 seconds as opposed to 46 seconds by \( W(u, \beta) \), i.e., \( W_1(u, \beta) \) is about 44 times slower than \( W(u, \beta) \). From now on, we use the \( W(u, \beta) \) function defined via Stehfest (1971) Laplace inversion algorithm.

4.3.3 Derivatives of the leaky well function, \( W(u, \beta) \)

Depending on the algorithm, parameter estimation from the dipole-flow test based on the upper-chamber drawdown measurements, should involve equations (8) or
(9) or (14) or (15) and their derivatives. Consequently, we need to define additionally

the derivatives of $W[u, \beta]$ defined by (2) and restated below:

$$W(u, \beta) = \int_{u}^{\infty} \frac{e^{-\frac{\beta y}{4}}}{y} \, dy$$

The derivative with respect to $u$ follows from the Leibnitz rule:

$$\frac{\partial}{\partial u} W(u, \beta) = \int_{u}^{\infty} \frac{\partial}{\partial u} \left( \frac{e^{-\frac{\beta y}{4}}}{y} \right) \, dy + \frac{e^{-\infty - \frac{\beta u}{4\infty}}}{\infty} \frac{\partial}{\partial u} \int_{u}^{\infty} \frac{e^{-\frac{\beta y}{4}}}{y} \, dy - \frac{e^{-u - \frac{\beta u}{4u}}}{u} \frac{\partial}{\partial u}$$

or

$$\frac{\partial}{\partial u} W(u, \beta) = - \frac{e^{-u - \frac{\beta u}{4u}}}{u}$$

Similarly,

$$\frac{\partial}{\partial \beta} W(u, \beta) = \int_{u}^{\infty} \frac{\partial}{\partial \beta} \left( \frac{e^{-\frac{\beta y}{4}}}{y} \right) \, dy + \frac{e^{-\infty - \frac{\beta u}{4\infty}}}{\infty} \frac{\partial}{\partial \beta} \int_{u}^{\infty} \frac{e^{-\frac{\beta y}{4}}}{y} \, dy - \frac{e^{-u - \frac{\beta u}{4u}}}{u} \frac{\partial}{\partial \beta}$$

or

$$\frac{\partial}{\partial \beta} W(u, \beta) = - \beta \int_{u}^{\infty} \frac{e^{-\frac{\beta y}{4}}}{2 y^2} \, dy$$

where we used the $\beta$ derivative of the integrand in (2):

$$D\left[ \frac{e^{-\frac{\beta y}{4}}}{y}, \beta \right]$$

$$- \frac{e^{-\frac{\beta y}{4}}}{2 y^2} \beta$$

As one can check, the integral in (19) does not have a closed form representation.

Indeed,
We expect that the definition of $\frac{\partial}{\partial \beta} W(u, \beta)$ via numerical integration will be relatively as inefficient as that of $W(u, \beta)$. Consequently, we define this derivative via numerical inversion of its Laplace transform. Recall representation (14), which we restate below

$$W(u, \beta) = \mathcal{L}^{-1}\left\{ \frac{2}{p} K_{0}\left(\sqrt{p + \beta^2}\right), p \to u \right\}$$

Differentiating with respect to $\beta$ we get:

$$\frac{\partial}{\partial \beta}\left[ p^2 BesselK\left[0, \sqrt{p + \beta^2}\right], \beta\right] \text{ FullSimplify}$$

$$\frac{2 \beta BesselK\left[1, \sqrt{p + \beta^2}\right]}{p \sqrt{p + \beta^2}}$$

$$\frac{\partial}{\partial \beta}\left[ p^2 BesselK\left[0, \sqrt{p + \beta^2}\right], \{\beta, 2\}\right] \text{ FullSimplify}$$

$$\left(2 \beta^2 \sqrt{p + \beta^2} BesselK\left[0, \sqrt{p + \beta^2}\right] + 2 (-p + \beta^2) BesselK\left[1, \sqrt{p + \beta^2}\right]\right)$$

$$\left(p \left(p + \beta^2\right)^{3/2}\right)$$

Hence

$$\frac{\partial}{\partial \beta} W(u, \beta) = -2 \beta \mathcal{L}^{-1}\left\{ \frac{1}{p \sqrt{p + \beta^2}} K_{0}\left(\sqrt{p + \beta^2}\right), p \to u \right\}$$

and

(20)
\[
\frac{\partial^2}{\partial \beta^2} W(u, \beta) =
\]
\[
\mathcal{L}^{-1}\left\{ \frac{1}{p(\beta^2 + p)^{3/2}} \left( 2\beta^2 \sqrt{\beta^2 + p} \ K_0(\sqrt{\beta^2 + p}) + 2(\beta^2 - p) K_1(\sqrt{\beta^2 + p}) \right) \right\},
\]
\[
p \to u \}
\]
The remaining two derivatives follow from (15)
\[
\frac{\partial}{\partial u} W(u, \beta) = -\frac{e^{-u - \beta}}{4u}
\]
\[
\text{D}\left[ -\frac{e^{-u - \beta}}{4u} \right], u \quad \text{FullSimplify}
\]
\[
e^{-u - \beta} \left( 4u (1 + u) - \beta^2 \right)
\]
\[
4u^3
\]
\[
\text{D}\left[ -\frac{e^{-u - \beta}}{4u} \right], \beta \quad \text{FullSimplify}
\]
\[
e^{-u - \beta} \frac{\beta}{2u^2}
\]
Hence,
\[
\frac{\partial^2}{\partial u^2} W(u, \beta) = \frac{e^{-u - \beta} \left( 4u (1 + u) - \beta^2 \right)}{4u^3}
\]
\[
\frac{\partial^2}{\partial u \partial \beta} W(u, \beta) = \frac{e^{-u - \beta} \beta}{2u^2}
\]
\[
\text{(22)}
\]
\[
\text{(23)}
\]

Conclusions for \(W[u, \beta]\) and its derivatives:

In our parameter estimation methodology, we use the following special functions:
\[ W(u, \beta) = L^{-1} \left\{ \frac{2}{p} K_o \left( \sqrt{p + \beta^2} \right), p \to u \right\} \]

\[ \frac{\partial}{\partial \beta} W(u, \beta) = L^{-1} \left\{ \frac{-2 \beta}{p \sqrt{p + \beta^2}} K_o \left( \sqrt{p + \beta^2} \right), p \to u \right\} \]

\[ \frac{\partial^2}{\partial \beta^2} W(u, \beta) = L^{-1} \]

\[ \left\{ \left( 2 \beta^2 \sqrt{\beta^2 + p} K_0 \left( \sqrt{\beta^2 + p} \right) + 2 (\beta^2 - p) K_1 \left( \sqrt{\beta^2 + p} \right) \right) \left/ \left( p (\beta^2 + p)^{3/2} \right) \right\}, p \to u \right\} \]

\[ \frac{\partial}{\partial u} W(u, \beta) = -\frac{e^{-u - \frac{\beta^2}{4u}}}{u} \]

\[ \frac{\partial^2}{\partial u^2} W(u, \beta) = \frac{e^{-u - \frac{\beta^2}{4u}} (4u (1 + u) - \beta^2)}{4u^3} \]

\[ \frac{\partial^2}{\partial u \partial \beta} W(u, \beta) = \frac{e^{-u - \frac{\beta^2}{4u}} \beta}{2u^2} \]

All these definitions are coded in our package Hantush.m.
Chapter 5: Example of Kabala (1993, p. 102) Revisited

5.1 Application of the Dipole-Flow Test Model:

Let us consider the same example as Kabala (1993, p. 102). We recast eq’n (9) in dimensionless form for confined aquifers ($\beta_w = 0$):

$$\frac{\pi K_r b s(t)}{Q} = \sum_{n=1}^{\infty} \left[ \frac{\sin \left( \frac{n \pi \Delta}{b} \right)^2}{\sin \left( \frac{n \pi}{2 b} \right)} \sin \left( \frac{n \pi}{2 b} \right) \sin \left( \frac{n \pi}{2 b} \right) \right]$$

$$\cos \left( \frac{n \pi}{b} \right) W \left( u_r, \frac{n \pi r_w}{a b} \right)$$

5.1.1 Parameters

Let us define first the dimensionless parameters

$$S = \frac{\pi K_r b s(t)}{Q} \quad \lambda = \frac{1}{b} \quad \beta = \frac{d}{b} \quad \delta = \frac{\Delta}{b} \quad \rho = \frac{r_w}{b} \quad \alpha = a^2 = \frac{K_r}{K_z}$$

Using the same values as Kabala (1993, p. 102), we have

$\lambda = 0.8; \beta = 0.4; \delta = 0.05; \rho = 0.01$;

We wish to plot the dimensionless drawdown as a function of dimensionless time, $1/u_r$,

for $\alpha = a^2 = 1, 2, 5, 10, \text{ and } 20$.

5.1.2 The Function

Definition of dimensionless drawdown function in terms of the leaky aquifer function $W$
\[
S[\tau, \alpha, M] := \sum_n \left( \frac{\sin \frac{n \pi \delta}{\tau}}{n \pi} \right)^2 \sin \left[ n \pi \frac{\lambda + \beta}{2} \right]
\]

\[
\sin \left[ n \pi \frac{\lambda - \beta - 2 \delta}{2} \right] \cos \left[ n \pi (\beta + \delta) \right] W \left[ 1 / \tau, \frac{n \pi \beta}{\sqrt{\alpha}} \right], \{n, 1, M\}
\]

\[
S[1000000, 10, 100] = 15.0039
\]

### 5.1.3 Series Cut-off Criterion

**Method 1**

Consider one value in the mid-range of function \( S \), and see how many terms we need to converge to it.

```mathematica
data = Table[S[1000, 20, 2*20 n]/S[1000, 20, 20 n], \{n, 1, 10\}];
\{1.03087, 1.01031, 1.0049, 1.00272, 1.00165, 1.00106, 1.00071, 1.00049, 1.00034, 1.00025\}

nn = Range[1, 10]; A = Transpose[{nn, data}];
ListPlot[A]
```

It seems that we need 100-200 terms.
Method 2
We will check whether or not increasing the number of terms in the Fourier series representation from, say, 100 to 200 makes an appreciable difference. As can be seen from the plot below, it doesn’t pay to do so.

\[
\text{S}[100, 5, 100] = 9.03706
\]

\[
\text{LogLinearPlot}\left[ \text{S}[^\tau, 5, 100] / \text{S}[^\tau, 5, 200], \{^\tau, 1, 10^5\} \right]
\]

Conclusions
We said earlier about 100 terms should suffice as the series terms likely alternate in sign. Indeed, this turns out to be the case.

Results
Let’s re-plot Kabala (1993, Fig. 2).
\[
p1 = \text{LogLinearPlot}
\]

Table[S[\tau, \alpha, 100], \{\alpha, \{1, 2, 5, 10, 20\}\}], \{\tau, 1, 10^5\}, \text{PlotRange} \to \{0, 20\}\]
Chapter 6: Parameter Estimation from the Dipole-Flow Test Model

6.1 The Dipole-Flow Test: Hypothetical Example of Kabala (1993, p. 102)

Here we consider an example similar to the one studied by Kabala (1993, p. 102) and later by Hvilshoj et al. (2000). A dipole-flow test is conducted on an upper chamber in an anisotropic, homogeneous, confined aquifer.

6.1.1 The Model

The drawdown in the upper chamber is described by equation (9) derived in section 4.2.1, and earlier reported by Kabala (1993, eqn 5). For a confined aquifer ($\beta_w = 0$) and $\Delta_u = \Delta_L = \Delta$, it reads:

$$s(t) = \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \sin\left(\frac{n \pi \Delta}{b}\right)^2 \sin\left(\frac{n \pi}{2} \frac{d+1}{2 b}\right) \sin\left(\frac{n \pi}{2} \frac{1-d-2 \Delta}{2 b}\right)$$

$$\cos\left(\frac{n \pi}{b} \frac{d+\Delta}{2}\right) W\left(u_r, \frac{n \pi r_w}{a b}\right)$$

(24)

where the variables have been defined earlier, $W(u, \beta)$ is the leaky aquifer function of Hantush (1961, 1964)

$$W(u, \beta) = \int_u^{\infty} \frac{y^{-u} e^{-y/4}}{y} dy$$

and

$$v_r = \frac{K_r}{S_s} \quad u_r = \frac{r_w^2}{4 v_r t} \quad a^2 = \frac{K_r}{K_z}$$
6.1.2 The Geometry and the Dipole-Flow System

We assume the same geometric parameters as in Kabala (1993, p. 102):

\[
\begin{align*}
\lambda &= \frac{1}{b} \\
\beta &= \frac{d}{b} \\
\delta &= \frac{\Delta}{b} \\
\rho &= \frac{r_w}{b}
\end{align*}
\]

\[
\lambda = 0.8; \beta = 0.4; \delta = 0.05; \rho = 0.01;
\]

Furthermore, we assume

\[
\begin{align*}
b &= 10 \, (\text{m}) \\
Q &= 0.00004 \, (\text{m}^3/\text{s})
\end{align*}
\]

\[
\gamma = \frac{r_w^2}{4} \, (\text{m}^2);
\]

\[
r_w = b \rho \, (\text{m});
\]

6.1.3 "True" Aquifer Parameters

The aquifer parameters that we typically need to estimate are horizontal hydraulic conductivity, \(K_r\), vertical hydraulic conductivity, \(K_z\), and specific storativity (or specific yield), \(S_s\). However, based on the form of our model, it is more convenient to select as our aquifer parameters the related triplet of \(\{\eta, K_r, a\}\):

\[
\eta = \frac{1}{\nu_f} = \frac{S_s}{K_r} \quad K = K_r \quad a = \sqrt{\frac{K_r}{K_z}}
\]

We also assume that our “true” aquifer parameters are

\[
K_r = K = 0.00001 \, (\text{m/s}) \; ; \; S_s = 0.0008 \, (1/\text{m}) \; ; \; a = \sqrt{10};
\]

With
\[ \eta = \frac{S_s}{K_r}; \]

the related “true” triplet is

\{\eta, K, a\}
\{80., 0.00001, 3.16228\}

Thus

\{S_s, K_r, a\} = \{\eta, K, a\}
\{0.0008, 0.00001, 3.16228\}

6.1.4 The Model, the Well Function and its Derivatives in Package

Hantush.m

The model, the well function \( W(u, \beta) \) and its derivatives are defined in the package

Hantush.m. Loading it is straightforward:

<< ~/teaching/advising/Michelle_Embon/Thesis/Hantush.m

\[ W[0.0001, .1] \]

4.85414

6.2 Generation of Hypothetical Measurements

Let us code the function (1) in terms of earlier defined parameters:
\[ s[t, \eta, K, a, M] := \frac{Q}{\pi K b} \sum \left[ \left( \frac{\sin(n \pi \delta)}{n \pi \delta} \right)^2 \sin\left( n \pi \frac{\lambda + \beta}{2} \right) \right. \]

\[ \left. \sin\left( n \pi \frac{\lambda - \beta - 2 \delta}{2} \right) \cos\left[ n \pi (\beta + \delta) \right] W\left[ y \eta / t, \frac{n \pi \rho}{a} \right], \{n, 1, M\} \right] \]

We use 100 terms in the series, which we found earlier to be sufficient:

### 6.2.1 Measurement Times

Let’s select times as a geometric progression

\[ t_0 = 0.1 \text{ (sec)}; \]

\[ \text{times} = \text{Table}\left[ t_0 \times 1.25^{i-1}, \{i, 1, 53\}\right]; \]

Assume that the measurement times are (in seconds):

\[ \text{times} = \text{Floor}\left[ 100 \times \text{times} \right] / 100. \]

\{0.1, 0.12, 0.15, 0.19, 0.24, 0.3, 0.38, 0.47, 0.59, 0.74, 0.93, 1.16, 1.45, 1.81, 2.27, 2.84, 3.55, 4.44, 5.55, 6.93, 8.67, 10.84, 13.55, 16.94, 21.17, 26.46, 33.08, 41.35, 51.69, 64.62, 80.77, 100.97, 126.21, 157.77, 197.21, 246.51, 308.14, 385.18, 481.48, 601.85, 752.31, 940.39, 1175.49, 1469.36, 1836.7, 2295.88, 2869.85, 3587.32, 4484.15, 5605.19, 7006.49, 8758.11, 10947.6\}  

### 6.2.2 "Exact" Drawdowns

The exact drawdowns follow from the model and the approximate measurement times.
\[ \text{drawdowns} = s \times \eta, K, a, 100 \]

\{ 0.015221861329794022', 0.02437508258228545', 0.04001842428768248', 0.06248265377087212', 0.09088705740788854', 0.12368532549352983', 0.16410341584546553', 0.20497071467598163', 0.2528615042130987', 0.30425499836709713', 0.3592166662501445', 0.41479332113390366', 0.4728431318968446', 0.5320245988540433', 0.5935961762098884', 0.655295561619154', 0.7172342237419753', 0.7795513960543159', 0.8417024448180601', 0.903362415301965', 0.965098425550321', 1.02608986709796', 1.0862454631550083', 1.1454894118928542', 1.203501137563823', 1.2602305803235103', 1.3155015468000983', 1.3690039403277954', 1.42056603248755', 1.469970545612051', 1.5169523029643313', 1.5613943051877945', 1.6031071456960806', 1.6420279734671737', 1.6780898174883339', 1.711297545202172', 1.7416634433695535', 1.769136810676856', 1.7938826841872395', 1.8157192498387813', 1.8347137932121311', 1.8509263839467562', 1.8644869121897243', 1.875593869572405', 1.884526025783729', 1.8915546736329765', 1.8969715640243845', 1.9010439117081557', 1.9040192823262194', 1.9061287432630731', 1.9075860126581794', 1.9085779292612197', 1.9092495435443941' \}

6.2.3 Measured Drawdowns within Errors of $\Delta s = 0.005 \text{ m} = 0.5 \text{ cm}$

drawdownsMeasured = Round[100 drawdowns]/100.

\{0.02, 0.02, 0.04, 0.06, 0.09, 0.12, 0.16, 0.2, 0.25, 0.3, 0.36, 0.41, 0.47, 0.53, 0.59, 0.66, 0.72, 0.78, 0.84, 0.9, 0.97, 1.03, 1.09, 1.15, 1.2, 1.26, 1.32, 1.37, 1.42, 1.47, 1.52, 1.56, 1.6, 1.64, 1.68, 1.71, 1.74, 1.77, 1.79, 1.82, 1.83, 1.85, 1.86, 1.88, 1.88, 1.89, 1.9, 1.9, 1.9, 1.9, 1.9, 1.9, 1.9, 1.9\}

Measurement Data (Times & Drawdowns)
dataMeasured = Transpose[{times, drawdownsMeasured},];
6.2.4 Assume the Aquifer Parameters are Unknown

We assume from now on that the aquifer parameters are unknown, and we will attempt to
Clear[η, K, a]

6.3 Parameter Estimation

We developed the parameter estimation procedure that consists of two steps:
- graphical parameter estimation and
- numerical parameter estimation.
The purpose of the former is to find a good initial estimation of the parameters which can then be used as initial guess in the latter step. The problem with numerical parameter estimation, and in particular with the Newton-Raphson scheme, is that the initial
guess has to be fairly close to the true values. In other words, the Newton-Raphson scheme has a small radius of convergence.

### 6.4 Graphical Parameter Estimation

#### 6.4.1 Parameter Estimation: Iteration # 1

Initial Guess for \( a^2 = \frac{K_r}{K_z} \)

Since typically the hydraulic conductivity ratio, \( a^2 = \frac{K_r}{K_z} \), ranges from 1 to 100, and \( a \) ranges from 1 to 10, we chose a midpoint value as our initial guess:

\( a = 5 \);

**K**\(_r\) from Steady-State Information

The steady-state drawdown follows from (1) as

\[
\begin{align*}
    s_\infty &= \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \left[ \frac{\sin(n\pi \frac{d + \Delta}{b})}{n\pi \frac{\Delta}{b}} \right]^2 \sin\left(n\pi \frac{d + 1}{2b}\right) \sin\left(n\pi \frac{1 - d - 2\Delta}{2b}\right) \\
    &\times \cos\left(n\pi \frac{d + \Delta}{b}\right) 2 K_o \left(\frac{n\pi r_w}{a b}\right)
\end{align*}
\]

Thus, given \( a \), the horizontal hydraulic conductivity is

\[
K_r = \frac{2 Q}{\pi s_\infty b} \sum_{n=1}^{\infty} \left[ \frac{\sin(n\pi \frac{\Delta}{b})}{n\pi \frac{\Delta}{b}} \right]^2 \sin\left(n\pi \frac{d + 1}{2b}\right) \sin\left(n\pi \frac{1 - d - 2\Delta}{2b}\right) \\
\times \cos\left(n\pi \frac{d + \Delta}{b}\right) K_o \left(\frac{n\pi r_w}{a b}\right)
\]

(25)

From the measurements we have
\[ s_\infty = 1.9 \ (\ast \ m \ast); \]

\[ K_{\text{fromSteady}}[a_, M_] := \frac{Q}{\pi s_\infty b} \sum \left( \frac{\sin(n\pi \delta)}{n\pi \delta} \right)^2 \sin \left( n\pi \frac{\lambda + \beta}{2} \right) \]

\[ \sin \left( n\pi \frac{\lambda - \beta - 2\delta}{2} \right) \cos \left( n\pi (\beta + \delta) \right) 2 \text{BesselK} \left[ 0, \frac{n\pi \rho}{a} \right], \{n, 1, M\} \]

Given \( a = 5 \), the estimate for the horizontal hydraulic conductivity is thus

\[ K = K_{\text{fromSteady}}[a, 100] \]

0.0000115402

(in m/s).

Corresponding Initial Estimate for \( \eta \)

We will find the initial guess for \( \eta \) graphically using our initial guesses for \( K \) and \( a \). Assume first

\[ S_s = 0.0001 \ (\ast \ 1/\mathrm{m} \ast); \ \eta = \frac{S_s}{K}; \]

\[ \text{InitialGuessParameters1} = \{\eta, K, a\} \]

\[ \{8.66536, 0.0000115402, 5\} \]

Given our initial guesses for \( \{\eta, K, a\} \), let’s generate the model drawdowns at the measurement times and plot them against the “true” measurements:

\[ \text{drawdownsFitted} = s[\text{times}, \eta, K, a, 100]; \]

\[ \text{dataFitted} = \text{Transpose}[\{\text{times}, \text{drawdownsFitted}\}]; \]

\[ \text{p2} = \text{ListLogLinearPlot}[\text{dataFitted}, \text{PlotStyle} \to \{\text{Red, PointSize}[\text{Large}]\}]; \]
Correction # 1 for $\eta$

Adjust the estimate of $S_s$, i.e., increase it to bring the body of the S-curve down, and repeat the process:

$$S_s = 0.0005 \times \frac{1}{m}; \quad \eta = \frac{S_s}{K};$$

InitialGuessParameters2 = \{$\eta$, K, a\}

\{43.3268, 0.0000115402, 5\}

drawdownsFitted = s[times, $\eta$, K, a, 100];

dataFitted = Transpose[{times, drawdownsFitted}];
p2 = ListLogLinearPlot[dataFitted, PlotStyle -> {Red, PointSize[Medium]}];
Correction # 2 for $\eta$

Adjust the estimate of $S_s$, i.e., **increase it to bring the body of the S-curve down**, and repeat the process:

$$S_s = 0.0007 \times (1/m); \quad \eta = \frac{S_s}{K};$$

InitialGuessParameters3 = \{\eta, K, a\}
\{60.6575, 0.0000115402, 5\}

drawdownsFitted = s\{times, \eta, K, a, 100\};
dataFitted = Transpose[{times, drawdownsFitted}];
p2 = ListLogLinearPlot[dataFitted, PlotStyle \rightarrow \{Red, PointSize[Large]\}];
Correction # 3 for $\eta$

Adjust the estimate of $S_s$, i.e., decrease it to bring the body of the S-curve slightly up, and repeat the process:

$$S_s = 0.0006 \times \frac{1}{m}; \quad \eta = \frac{S_s}{K}$$

InitialGuessParameters3 = \{\eta, K, a\}  
\{51.9922, 0.0000115402, 5\}

drawdownsFitted = s[times, \eta, K, a, 100];

dataFitted = Transpose[{times, drawdownsFitted}];

p2 = ListLogLinearPlot[dataFitted, PlotStyle -> {Red, PointSize[Large]}];
Conclusions

The initial best estimates for the parameters are those from Correction # 3, i.e.,

\[ S_s = 0.0006 \text{ (* 1/m *)}; \quad \eta = \frac{S_s}{K}; \]

Hence, our initial best estimates for the aquifer parameters are

\[
\text{bestParameters} = \{ \eta, K, a \} = \{51.9922, 0.0000115402, 5\}
\]

6.5 Derivation of the Newton-Raphson Scheme

Consider a vector function

\[ F[x^*] = 0 \]

We can find its unknown vector root, \( x^* \), from an initial guess vector, \( x \), by expanding this function in Taylor series around the initial guess and by dropping all higher order terms. With

\[ (x^* - x) = \Delta x \]

we have
\[ 0 = F[x^*] = F[x + (x^* - x)] = F[x + \Delta x] \approx F[x] + \frac{\partial F[x]}{\partial x} \Delta x \]

where \( \frac{\partial F[x]}{\partial x} \) is the Jacobian matrix.

Thus
\[ \Delta x \approx -\left( \frac{\partial F[x]}{\partial x} \right)^{-1} F[x] \]

and
\[ x^* = x - \left( \frac{\partial F[x]}{\partial x} \right)^{-1} F[x] \]

where \( \left( \frac{\partial F[x]}{\partial x} \right)^{-1} \) is the pseudoinverse of the Jacobian matrix \( \frac{\partial F[x]}{\partial x} \).

Since we dropped the higher order terms in the Taylor expansion, the derived relationship is only approximate. The Newton-Raphson scheme iterates on this relation from an initial guess \( x_o \):
\[ x_{n+1} = x_n - \left( \frac{\partial F[x_n]}{\partial x} \right)^{-1} F[x_n] \]

When the process converges, the resulting root represents the least-square fit to the data.

**NOTE:** The Newton-Raphson scheme is second order, i.e., if it does converge, it does it rapidly. Its main problem is a relatively small radius of convergence, i.e., the need to have a very good initial guess.

Let the \( i \)-th drawdown measurement, \( s_i \), be one conducted at the \( i \)-th time, \( t_i \):
\[ F_i[\{\eta, K, a\}] = -s_i + f(t_i, \eta, K, a) \quad (26) \]

where the function \( f(t_i, \eta, K, a) \) is such as (1), (4), (5), or (6). Here we assume that this function is that given by (15).

The function \( F_i \) should be zero when the parameter vector \( \{\eta, K, a\} \) is equal to the true values. But during the iterative process it will not be zero.

The Jacobian matrix is thus defined by
\[
\frac{\partial F}{\partial x} = \begin{pmatrix}
\frac{\partial F_1}{\partial \eta} & \frac{\partial F_1}{\partial K} & \frac{\partial F_1}{\partial a} \\
\vdots & \vdots & \vdots \\
\frac{\partial F_i}{\partial \eta} & \frac{\partial F_i}{\partial K} & \frac{\partial F_i}{\partial a} \\
\vdots & \vdots & \vdots \\
\frac{\partial F_1}{\partial \eta} & \frac{\partial F_1}{\partial K} & \frac{\partial F_1}{\partial a}
\end{pmatrix}
\]  

(27)

Let’s be more specific. Again, our initial best estimates for the aquifer parameters are

Now, from (15) and (17), we have

\[
\frac{\partial F_i}{\partial \eta} = \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \left( \frac{\sin(n\pi \delta)}{n\pi \delta} \right)^2 \sin\left[ n\pi \frac{\lambda + \beta}{2} \right] \sin\left[ n\pi \frac{\lambda - \beta - 2\delta}{2} \right]
\]

(28)

\[
\cos[n\pi (\beta + \delta)] \frac{\partial W[\gamma \eta / t_i, n\pi \rho_a]}{\partial u} \frac{\gamma}{t_i}
\]

\[
\frac{\partial F_i}{\partial K_r} = -\frac{1}{K_r} \left( \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \left( \frac{\sin(n\pi \delta)}{n\pi \delta} \right)^2 \sin\left[ n\pi \frac{\lambda + \beta}{2} \right] \sin\left[ n\pi \frac{\lambda - \beta - 2\delta}{2} \right] \right)
\]

(29)

\[
\frac{\partial F_i}{\partial a} = \frac{Q}{\pi K_r b} \sum_{n=1}^{\infty} \left( \frac{\sin(n\pi \delta)}{n\pi \delta} \right)^2 \sin\left[ n\pi \frac{\lambda + \beta}{2} \right] \sin\left[ n\pi \frac{\lambda - \beta - 2\delta}{2} \right]
\]

\[
\cos[n\pi (\beta + \delta)] \frac{\partial W[\gamma \eta / t_i, n\pi \rho_a]}{\partial \beta} \left( -\frac{n\pi \rho}{a^2} \right)
\]

(30)

Note that we do not need to define \( \frac{\partial F_1}{\partial K_r} \) as this is simply equal to \( -\frac{1}{K_r} s \), but let us define the corresponding derivatives, \( \frac{\partial F_1}{\partial \eta} \) and \( \frac{\partial F_1}{\partial a} \).
\[
\text{dFdeta}[t\_, \eta\_, K\_, a\_, M\_] := \\
\frac{Q}{\pi K b} \sum \left( \frac{\sin[n \pi \delta]}{n \pi \delta} \right)^2 \sin\left[ n \pi \frac{\lambda + \beta}{2} \right] \sin\left[ n \pi \frac{\lambda - \beta - 2 \delta}{2} \right] \\
\cos[n \pi (\beta + \delta)] d1du1W\left[ \gamma \frac{\eta}{t}, \frac{n \pi \rho}{a} \right] \left[ \frac{\gamma}{t}, \{n, 1, M\} \right]
\]

\[
\text{dFda}[t\_, \eta\_, K\_, a\_, M\_] := \\
\frac{Q}{\pi K b} \sum \left( \frac{\sin[n \pi \delta]}{n \pi \delta} \right)^2 \sin\left[ n \pi \frac{\lambda + \beta}{2} \right] \sin\left[ n \pi \frac{\lambda - \beta - 2 \delta}{2} \right] \\
\cos[n \pi (\beta + \delta)] d1db1W\left[ \gamma \frac{\eta}{t}, \frac{n \pi \rho}{a} \right] \left[ \frac{-n \pi \rho}{a^2}, \{n, 1, M\} \right]
\]

With these functions, we can now define the Jacobian \( \frac{\partial F}{\partial x} \) as a matrix named dFdx.

\textbf{6.6 Newton-Raphson Scheme with Full Data}

Here we use the parameter estimates from the previous stage (Graphical Estimates) to serve as our initial guess.

Computational Iteration \# 1

\{\eta, K, a\} = bestParameters;

drawdownsFitted = s[times, \eta, K, a, 100];

F = -drawdowns + drawdownsFitted;
\[ \text{dFdx} = \text{Table}\left(\left\{ \text{dFdeta}[\text{times}[[i]], \eta, K, a, 100], \frac{-1}{K} s[\text{times}[[i]], \eta, K, a, 100], \text{dFda}[\text{times}[[i]], \eta, K, a, 100]\right\}, \{i, 1, \text{Length[times]}\}\right); \]

\[ \{\eta, K, a\} = \{\eta, K, a\} - \text{PseudoInverse}[\text{dFdx}] F \]

\[ \{74.9424, 9.9574 \times 10^{-6}, 2.64605\} \]

**Computational Iteration # 2**

\[ \text{drawdownsFitted} = s[\text{times}, \eta, K, a, 100]; \]

\[ F = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left(\left\{ \text{dFdeta}[\text{times}[[i]], \eta, K, a, 100], \frac{-1}{K} s[\text{times}[[i]], \eta, K, a, 100], \text{dFda}[\text{times}[[i]], \eta, K, a, 100]\right\}, \{i, 1, \text{Length[times]}\}\right); \]

\[ \{\eta, K, a\} = \{\eta, K, a\} - \text{PseudoInverse}[\text{dFdx}] F \]

\[ \{78.9984, 0.0000100692, 3.1621\} \]

**Computational Iteration # 3**

\[ \text{drawdownsFitted} = s[\text{times}, \eta, K, a, 100]; \]

\[ F = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left(\left\{ \text{dFdeta}[\text{times}[[i]], \eta, K, a, 100], \frac{-1}{K} s[\text{times}[[i]], \eta, K, a, 100], \text{dFda}[\text{times}[[i]], \eta, K, a, 100]\right\}, \{i, 1, \text{Length[times]}\}\right); \]

\[ \{\eta, K, a\} = \{\eta, K, a\} - \text{PseudoInverse}[\text{dFdx}] F \]

\[ \{79.9971, 9.99968 \times 10^{-6}, 3.16243\} \]
Computational Iteration # 4

drawdownsFitted = s[times, \eta, K, a, 100];

F = -drawdowns + drawdownsFitted;

dFdx = Table[{-1 \frac{s[times[i], \eta, K, a, 100]}{K}, dFda[times[i], \eta, K, a, 100]}, {i, 1, Length[times]}];

{\eta, K, a} = {\eta, K, a} - PseudoInverse[dFdx].F

{80., 0.00001, 3.16228}

Note that despite the fact that we have truncated the “true” measurement, each one within 0.5 cm error, we were able to recover the exact “true” parameters.

Final Plot

dataFitted = Transpose[{times, drawdownsFitted}];

p2 = ListLogLinearPlot[dataFitted, PlotStyle -> {Red, PointSize[Large]}];

Show[p1, p2]
Final Parameters
The final estimated parameters are
\{\eta, K, a\} = \{80., 0.00001, 3.16228\}
Thus the “true” parameters (see above) are:
\{S_s, K_r, a\} = \{\eta K, K, a\} = \{0.0008, 0.00001, 3.16228\}

6.7 Question: Can the initial guess be further off?

Recall our first guess of the aquifer parameters was based on the assumption that
\(a = 5\). Let’s start with an even poorer guess of \(a = 10\), i.e., \(a^2 = K_r / K_z = 100\), a full
order of magnitude larger than the “true” value of \(a^2 = 10\). Recall also the value of the
steady-state drawdown:
\(a = 10; s_\infty = 1.9\) (* m *);
The corresponding estimate for the horizontal hydraulic conductivity is thus
\[ K = K_{\text{fromSteady}}[a, 100] \]
0.000013804

We again assume \( S_s = 0.0001 \) (1/m), which is 8 times smaller than the “true” value:
\[ S_s = 0.0001 \text{ (1/m)}; \eta = \frac{S_s}{K} \]
7.24427
\{\eta, K, a\}
\{7.24427, 0.000013804, 10\}

The model predicted dipole-flow response is even further from the measured values:
drawdownsFitted = s[times, \eta, K, a, 100];
dataFitted = Transpose[[times, drawdownsFitted]]; p2 = ListLogLinearPlot[dataFitted, PlotStyle -> {Red, PointSize[Large]}]; Show[p1, p2]

The computational algorithm converges again in 5-6 iterations.
Computational Iteration # 1

drawdownsFitted = s[times, \eta, K, a, 100]; F = -drawdowns + drawdownsFitted;

dFdx = Table[{dFdeta[times[[i]], \eta, K, a, 100], \frac{-1}{K} s[times[[i]], \eta, K, a, 100], dFda[times[[i]], \eta, K, a, 100]}, {i, 1, Length[times]}];

{\eta, K, a} = {\eta, K, a} - PseudoInverse[dFdx].F

{24.0873, 0.0000110341, 2.15813}

Computational Iteration # 2

drawdownsFitted = s[times, \eta, K, a, 100]; F = -drawdowns + drawdownsFitted;

dFdx = Table[{dFdeta[times[[i]], \eta, K, a, 100], \frac{-1}{K} s[times[[i]], \eta, K, a, 100], dFda[times[[i]], \eta, K, a, 100]}, {i, 1, Length[times]}];

{\eta, K, a} = {\eta, K, a} - PseudoInverse[dFdx].F

{39.9778, 0.0000132189, 4.72765}
Computational Iteration # 3

\[ \text{drawdownsFitted} = s\{\text{times, } \eta, \text{K, a, 100}\}; F = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left[\left\{\text{dFdeta}\{\text{times[[i]], } \eta, \text{K, a, 100}\}, \frac{-1}{K} s\{\text{times[[i]], } \eta, \text{K, a, 100}\}, \text{dFda}\{\text{times[[i]], } \eta, \text{K, a, 100}\}\right\}, \{i, 1, \text{Length[times]}\}\right]; \]

\[ \{\eta, \text{K, a}\} = \{\eta, \text{K, a}\} - \text{PseudoInverse[}\text{dFdx}.\text{F} \]

\[ \{71.5148, 9.37015 \times 10^{-6}, 2.76005\} \]

Computational Iteration # 4

\[ \text{drawdownsFitted} = s\{\text{times, } \eta, \text{K, a, 100}\}; F = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left[\left\{\text{dFdeta}\{\text{times[[i]], } \eta, \text{K, a, 100}\}, \frac{-1}{K} s\{\text{times[[i]], } \eta, \text{K, a, 100}\}, \text{dFda}\{\text{times[[i]], } \eta, \text{K, a, 100}\}\right\}, \{i, 1, \text{Length[times]}\}\right]; \]

\[ \{\eta, \text{K, a}\} = \{\eta, \text{K, a}\} - \text{PseudoInverse[}\text{dFdx}.\text{F} \]

\[ \{78.2869, 0.0000100158, 3.15409\} \]
Computational Iteration # 5

drawdownsFitted = s[times, η, K, a, 100]; F = -drawdowns + drawdownsFitted;

dFdx = Table[{dFeta[times[[i]], η, K, a, 100], -1/K s[times[[i]], η, K, a, 100],

dFda[times[[i]], η, K, a, 100]}, {i, 1, Length[times]}];

{η, K, a} = {η, K, a} – PseudoInverse[dFdx].F
{79.973, 0.0000100005, 3.16278}

Computational Iteration # 6

drawdownsFitted = s[times, η, K, a, 100]; F = -drawdowns + drawdownsFitted;

dFdx = Table[{dFeta[times[[i]], η, K, a, 100], -1/K s[times[[i]], η, K, a, 100],

dFda[times[[i]], η, K, a, 100]}, {i, 1, Length[times]}];

{η, K, a} = {η, K, a} – PseudoInverse[dFdx].F
{79.999955648153`, 9.9999998891419`*^-6, 3.162277739409001`}

6.8 Question: Can the initial guess be way off?

Let’s start with an unreasonably poor guess of a = 11, i.e., a² = K_x / K_z = 144,
a full order of magnitude larger than the “true” value of a² = 10. Recall also the value
of the steady-state drawdown:

a = 11; s_∞ = 1.9 (± m ±);
The corresponding estimate for the horizontal hydraulic conductivity is thus
\[ K = K_{\text{from Steady}}[a, 100] \]
0.0000141161

We again assume \( S_s = 0.0001 \ (1/m) \), which is 8 times smaller than the “true” value:
\[ S_s = 0.0001 (\ast \ 1/m \ast); \quad \eta = \frac{S_s}{K} \]
7.08411
\{\eta, K, a\}
\{7.08411, 0.0000141161, 11\}

The model predicted dipole-flow response is way off the measured values--there is no S-curve quality to the predicted response:
\[ \text{drawdownsFitted} = s[\text{times}, \eta, K, a, 100] \];
\[ \text{dataFitted} = \text{Transpose}[\{\text{times, drawdownsFitted}\}] \];
\[ p2 = \text{ListLogLinearPlot}[\text{dataFitted, PlotStyle} \rightarrow \{\text{Red, PointSize}\{\text{Large}\}\}; \text{Show}[p1, p2] \]

The computational algorithm converges again in 5-6 iterations.
Computational Iteration # 1

\[ \text{drawdownsFitted} = s[times, \eta, K, a, 100]; \quad \text{F} = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left\{ \text{dFdeta[times[[i]], \eta, K, a, 100]}, -\frac{1}{K} s[times[[i]], \eta, K, a, 100], \text{dFda[times[[i]], \eta, K, a, 100]} \right\}, \{i, 1, \text{Length[times]}\}; \]

\[ \{\eta, K, a\} = \{\eta, K, a\} - \text{PseudoInverse[dFdx].F} \]

\[ \{24.2178, 0.0000108193, 0.658595\} \]

Computational Iteration # 2

\[ \text{drawdownsFitted} = s[times, \eta, K, a, 100]; \quad \text{F} = -\text{drawdowns} + \text{drawdownsFitted}; \]

\[ \text{dFdx} = \text{Table}\left\{ \text{dFdeta[times[[i]], \eta, K, a, 100]}, -\frac{1}{K} s[times[[i]], \eta, K, a, 100], \text{dFda[times[[i]], \eta, K, a, 100]} \right\}, \{i, 1, \text{Length[times]}\}; \]

\[ \{\eta, K, a\} = \{\eta, K, a\} - \text{PseudoInverse[dFdx].F} \]

\[ \{-12.8604, 0.000036385, 4.55615\} \]

Unfortunately, with \( a = 11 \), the scheme diverges.
Chapter 7: Future Recommendations

7.1 Recommendations for Future Research

With the robust model of transient dipole-flow test and associated parameter estimation procedure we are ready to analyze the unexplored data troves from numerous dipole-flow tests, conducted on the vertical-circulation wells constructed for aquifer remediation all over this country. This research would examine how well our modeled drawdowns and other parameters relate to the ones actually observed in the field testing. It would also further our understanding of how behaves under several varying parameters. For starters, we would like to explore the uninterpreted tests reported by Johnson and Simon (2007). Due to time constraints we were unable to conduct a full analysis of this data, but were able to initialize the exploration.

7.2 Dipole Flow Test at Cape Canaveral (2001)

The study was conducted near Facility 1381 at Cape Canaveral Air Station, Florida. This location had been targeted because of its elevated concentration of trichlorethylene within groundwater. The water recirculating wells contained an inside diameter (ID) of 0.15 meters. Within the packer, the upper chamber was 1.5 m long, extending from 1.5 to 3 m below the ground surface. It was installed fairly close to the water table in order to maximize the distance between the two screens. The lower
packer was twice its length, at 3.0 m, and extended from 6 to 9 m below the ground surface. It rested just below a highly contaminated zone. The two piezometers utilized to measure water pressure held an inside diameter of 0.032 m and extended for 0.5 m. One was placed 2 m below ground surface, and the second at 7.5 m. An additional 4 sets of 1 m long, 0.032 m ID piezometers were installed around the direct perimeter of the recirculation well.

Seven HydrotechnicsTM groundwater velocity sensors were mounted along two tangential paths from the well. Three of these were placed at a shallow depth of about 2 m bgs, while the remaining four were installed at a deeper 5m bgs. Measurements from these velocity sensors were collected every 2 minutes and stored on a Campbell Scientific CR-10 data logger. As a means of reinforcing the analysis and understanding of the site, an additional 80 microwells were installed in 20 nests along three transects across the site. Both pumping and slug tests were conducted prior to beginning the experiment in order to set control parameters for future site testing and evaluation. Specifically, the slug tests consisted of measuring the static head in the well, then introducing an almost instantaneous variation in water level, and gauging the change in water level over time until the level returned to the original static level.

Lastly, groundwater samples for TCE analysis was taken and analyzed with gas chromatography. In order to deepen the understanding of groundwater flow, two tracer solutions, hexafluoride and sodium fluorescein, were selected due to their low toxicity,
minimal biodegradation, and restricted sorption through porous media. These solutions were injected into the more shallow piezometers immediately outside of the well in order to prevent air stripping from the air pumping mechanism. The recirculation tracer test, for which the hexafluoride was used, estimated the percentage of water that flows directly from the upper screen outlet to the lower screen inlet of the recirculation well. A second test, the divergent tracer test, was implemented to observe the radius of movement traveling from the well through the surrounding aquifer.

7.3 Digitized Data from Johnson & Simon (2007)

Since the raw data from the experiment was not available either through the private engineering contractor or the EPA Technical Evaluation Report, all values were extracted from Johnson and Simon (2007) via the digitizing of relevant graphs. Numerous attempts were made to contact these entities throughout the greater part of the research year, yet we were ultimately unable to get the raw data from any of the people involved in this study.

7.3.1 Plot Digitizer

Plot Digitizer was primarily employed throughout most of the data recovery process. This Java-created program digitizes scanned plots/images of functional data,
and works with both linear and logarithmic axis scales. This software includes features that made it optimal for our tasks. For instance, it permitted for the recalibration of the X or Y axis with minimal interference. The program brought our individual data approximation to a precision level of .0001 decimal places. This process of data digitalization began by obtaining both scanned and photographed copies of all of the graphs contained in the Johnson & Simon article. They were then uploaded into the Plot Digitizer software, adjusting the zoom in order to maximize the visual integrity of each figure. Once in the platform, the data points within each table were calibrated by locating the corresponding X and Y axes and mirroring them within the digitizing virtual plot. This step allowed for the actual axis and the virtual one to superimpose and become near identical. After this step was completed we then proceeded to selected various points within each graph for digitizing (usually between 50 to 70). Once the coordinates of these were obtained we extracted them and plotted them utilizing the Mathematica software.

**7.3.2 Promising Unexplored Data from Johnson and Simon (2007)**

Although most of the data published by Johnson and Simon (2007) are hopelessly noisy, some are quite smooth and worthy of interpretation. They include:
Figure 1 - Graphical representation of the hydraulic head within piezometer 2PZ.

Figure 2 - Graphical representation of the vertical velocity within micro well C 4.
Figure 3 - Graphical representation of the hydraulic head within the groundwater circulation well.

Figure 3 - Site plan view of drawing of the site showing the location of the piezometers, flow sensors, and groundwater circulation well (modified from Johnson & Simon, 2007)

7.3.3 Future Interpretation of the Digitized Data

The data that we gathered from this field testing experiment has so far been vastly unexplored. No other research group has utilized this wide array of information to test their hydrological models. My graduate successor may wish to extract useful portions of the digitized data and interpret it. I will be happy to assist.
Chapter 8: Conclusion

8.1 Model for a Asymmetric Dipole Flow under Transient Conditions

We successfully present a mathematical model for determining the drawups and drawdowns of homogeneous aquifers under a dipole flow test containing asymmetrical chamber sizes. Our re-derivation and generalization of the existing dipole flow model enables us to use this aquifer characterization technique even when the anisotropy ration in over 1.

8.2 Development of a Parameter Estimation Technique

In this thesis we developed a two stage parameter estimation techniques based on our model. The two stages are graphical and numerical. In the geographical stage, we set initial investigational estimates for three crucial aquifer parameters (Kr, Kz, Ss) in hopes that they will produce similar responses to the ones found within field testing. Subsequently, in the numerical stage, we implement the Newton-Raphson algorithm to refine our initial values for the three parameters

8.3 Testing of the Parameter Estimation on Hypothetical Cases
We were successful at testing this parameter estimation technique on a synthetic/hypothetical example and to demonstrating its robustness.
### Appendix A: Notation and Units

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<thead>
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<th>Notation</th>
<th>Description</th>
<th>Units</th>
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<td>-</td>
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<td>K</td>
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<td>m/day</td>
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<tr>
<td>K_r</td>
<td>Horizontal hydraulic Conductivity</td>
<td>m/day</td>
</tr>
<tr>
<td>K_z</td>
<td>Vertical Hydraulic Conductivity</td>
<td>m/day</td>
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<td>Discharge Rate</td>
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<td>m</td>
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<td>W</td>
<td>Hantush Well Function</td>
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<td>sec.</td>
</tr>
<tr>
<td>Erf</td>
<td>Error Function</td>
<td>-</td>
</tr>
</tbody>
</table>
Appendix B: Trigonometric Identities

Identity #1

We derive here a trigonometric identity for the difference of sines that we encounter in our derivation of equations for the dipole-flow test. We start with:

\[ e^{i(\alpha + \beta)} = e^{i\alpha} e^{i\beta} \]

and apply Euler’s identity:

\[ \cos(\alpha + \beta) + i \sin(\alpha + \beta) = (\cos(\alpha) + i \sin(\alpha))(\cos(\beta) + i \sin(\beta)) \]

Now comparing the imaginary parts of both sides, we get

\[ \sin(\alpha + \beta) = \sin(\alpha) + \cos(\beta) + \sin(\beta) + \cos(\alpha) \]

Changing \( \beta \) to \(-\beta\) in the above equation and employing the fact that sine is an odd function while cosine is an even function, we get

\[ \sin(\alpha - \beta) = \sin(\alpha)\cos(\beta) - \sin(\beta)\cos(\alpha) \]

Subtracting the last equation from the penultimate one, yields

\[ \sin(\alpha + \beta) - \sin(\alpha - \beta) = 2\sin(\beta)\cos(\alpha) \]

And finally, renaming the variables \( x = \alpha + \beta \) and \( y = \alpha - \beta \) (or \( \alpha = (x + y)/2 \) and \( \beta = (x - y)/2 \)), we get

\[ \sin(x) - \sin(y) = 2\sin\left(\frac{x - y}{2}\right)\cos\left(\frac{x + y}{2}\right) \]

Identity #2

Following the same first two steps of the previous derivation, we now compare the real parts of both sides, we get

\[ \cos(\alpha + \beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta) \]
Changing $\beta$ to $-\beta$ in the above equation and employing the fact that sine is an odd function while cosine is an even function, we get

$$\cos(\alpha - \beta) = \cos(\alpha)\cos(\beta) + \sin(\alpha)\sin(\beta)$$

Now, subtracting the penultimate equation from the last one, yields

$$\cos(\alpha - \beta) - \cos(\alpha + \beta) = 2\sin(\alpha)\sin(\beta)$$

And finally, renaming the variables $x = \alpha + \beta$ and $y = \alpha - \beta$ (or $\alpha = (x + y)/2$ and $\beta = (x - y)/2$), we get

$$\cos(y) - \cos(x) = 2\sin\left(\frac{x + y}{2}\right)\sin\left(\frac{x - y}{2}\right)$$
Appendix C: Hantush.m Mathematica Package

BeginPackage["Hantush"]
(* This package computes the well function and its derivatives for leaky aquifers *)
d2db2W::usage = " gives the values of ..."
d2du2W::usage = " gives the values of ..."
d2duldb1W::usage = " gives the values of ..."
d1db1W::usage = " gives the values of ..."
d1dulW::usage = " gives the values of ..."
W::usage = "W[u,\[Beta]] gives the values of the leaky-aquifer well function (Hantush, 1961, 1964)"

Begin["Hantush\`private"]

Wsteh[i_,M_] := (-1)^(M/2+i) Sum[
  k^(M/2) (2 k)! / ( (M/2 - k)! k! (i-k)! (2 k - i)! ),
  {k,Floor[(i+1)/2],Min[i,M/2]} ]

Vsteh[M_] := Table[Wsteh[i,M],{i,M}]

NN=16

ln2= Log[2]

V=Vsteh[NN]

Vabs=Abs[V]
Vmax=Max[V]
Vmin=Min[Vabs]
Vspan=Vmax/Vmin
Nsignif=Ceiling[N[Log[10,Vspan]]]

Nsignif=16

LW[p_,\[Beta]_] := 2 BesselK[0,Sqrt[p+\[Beta]^2]]/p

W[u_,\[Beta]_] := N[  ln2 4 u Sum[V[[i]]] LW[i ln2 4 u,\[Beta]],{i,1,NN}], Nsignif]

Ld2db2W[p_,\[Beta]_] := (2*\[Beta]^2*Sqrt[\[Beta]^2 + p]*BesselK[0, Sqrt[\[Beta]^2 + p]] + 2*(\[Beta]^2 - p)*BesselK[1, Sqrt[\[Beta]^2 + p]])/(p*(\[Beta]^2 + p)^(3/2))


Ld1db1W[p_,\[Beta]_] := -(2 \[Beta] BesselK[1, Sqrt[p + \[Beta]^2]])/(p Sqrt[p + \[Beta]^2]))

ld1db1W[u_,\[Beta]_] := N[  ln2 4 u Sum[V[[i]]] Ld1db1W[i ln2 4 u,\[Beta]],{i,1,NN}], Nsignif]
(* d1db1W[u_, \[Beta]_] := NIntegrate[-(E^(-y - \[Beta]^2/(4 y)) \[Beta])/(2 y^2)), {y, u, \[Infinity]}] *)

d2du2W[u_, \[Beta]_] := (E^(-u - \[Beta]^2/(4*u))*(4*u*(1 + u) - \[Beta]^2))/(4*u^3)

d2duldb1W[u_, \[Beta]_] := (E^(-u - \[Beta]^2/(4*u))*\[Beta])/(2*u^2)

dldulW[u_, \[Beta]_] := -(E^(-u - \[Beta]^2/(4*u))/u)

(*
Lmyf[p_] := 1/p

myf[t_] := N[ln2/t Sum[V[[i]] Lmyf[i ln2/t],{i,1,NN}], Nsignif]*

(* Plot[myf[t],{t,.001,100},PlotRange->{0,2}] *) *)

(* REFERENCES *)

End[]
EndPackage[]
References


