ANALYSIS OF EXACT GROUNDWATER MODEL WITHIN A CONFINED AQUIFER.

Mashudu Clifford Mathobo

Student Number: 2016113298

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Supervisor: Prof. Abdon Atangana

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DECLARATION

I, Mashudu Clifford Mathobo, declare that the thesis hereby submitted by me for the Magister Scientiae degree at the University of the Free State (Institute for Groundwater Studies), is my own independent work and has not previously been submitted by me at another university/ faculty.

I further declare that all sources cited or quoted are indicated and acknowledged by means of a list of references.

I furthermore cede copyright of the thesis in favor of the University of the Free State.

In addition, the following article has been submitted and is under review at an International Accredited Journal:

1. Mathobo, M.C. and Atangana, A., 2017. Analysis of Exact Groundwater Model within a Confined Aquifer: Beyond Theis Model

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LIST OF GREEK NOTATIONS

α	alpha
β	beta
τ	tau
∂	Partial Differentiation
δ	delta
φ	phi
Γ	Gamma
Δ	Delta
θ	delta
ϕ	phi
Φ	Phi
σ	Sigma
Σ	Sigma
μ	mu
$\mathcal{L}$	Laplace Transform

ABBREVIATIONS AND NOTATIONS

h	Hydraulic Head
r	Radial Distance
K	Hydraulic Conductivity
S	Storativity
S_s	Specific Storage
S_y	Specific Yield
T	Transmissivity
t	Time
q	Darcy Flux
Q	Discharge
V	Volume
c	Arbitrary Constant
r_b	Ratio of the Borehole
Δr	Scaling Constant
f	Function

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CHAPTER 1: INTRODUCTION

1.1 BACKGROUND OF THE STUDY

According to Fetter (1998) a model is “any representation of a real system”. (Bedient *et al.,* 1997) stated that “a ground water model is a tool designed to represent a simplified version of a real field site”. (Anderson and Woesner, 2002) agree by defining a model as “any device that represents an approximation of a field situation. (Mary *et al*., 2015) further stated that “a more powerful ground water model is one that quantitatively represents heads in space and time in a simplified representation of the complex hydrogeologic conditions in the subsurface”. The most common purpose of a model is to forecast the effects of some future action or hydrologic condition, but models are also used to re-create past conditions (hindcasting) and also as interpretive tools (Mary *et al*., 2015). According to Reilly and Harbough (2004), there are five broad categories of problems for ground water modelling: basic understanding of ground water systems; estimation of aquifer properties; understanding the present; understanding the past; and forecasting the future.

Ground water models can be divided into physical or mathematical models but for the sole purpose of this research, only mathematical models will be focused on. Mathematical models use equations to represent the process occurring in a field situation and include analytical, numerical and stochastic models (Fetter, 1998). Analytical models require a high level of simplification of the natural world in order to define a problem that can be solved mathematically to obtain a closed-form solution. Analytical solutions can be solved using a hand calculator but more complex solutions use a spreadsheet or computer program (Barlow and Moench, 1998). A model is stochastic if any of its parameters have a probabilistic distribution. Ground water modelling starts with the equation of flow. Two-dimensional groundwater flow in a confined aquifer with transmissivity T and storativity S is given as:

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}.\frac{\partial h}{\partial r} = \frac{S}{T}\frac{\partial h}{\partial t} \qquad (1.1)$$

Where h is the hydraulic head, S is storativity, T is the transmissivity, t is time, and r is the radial distance from the pumping well. Ground water movement is described by a group of simplified water flow governing equations; the predictions of ground water systems always deviate from observations. Therefore, the uncertainty of ground water simulation is inevitable.

As with any model (e.g. physical), mathematical models are associated with uncertainties. According to JiChun and XianKui (2013) uncertainty can be interpreted as “the lack of certainty, that is, a future or existing state cannot be described accurately because of limited information”. Numerous authors have inconsistently classified uncertainty sources of ground water. (Yen *et al*., 1986) classified modelling uncertainty into five parts: the natural uncertainty caused by the inherent randomness of natural process; the model uncertainty stemmed from defective model which is not able to represent the real physical process; the uncertainty of model parameter; the uncertainty from observation error; and the operating uncertainty cause by human factors. (Van Asselt, 2000) proposed that the uncertainty sources could be cognized at three levels that are generation location, managing level and natural quality respectively. (Liu and Shu, 2000) stressed that, according to discipline nature, the source could be interpreted as stochastic, fuzzy, gray, and unknown uncertainties. (Merz and Thieken, 2009) classified modelling uncertainties as aleatory and epistemic uncertainties. Recently, Hepburn (2011) classified modelling uncertainties into three general sources which are model parameter, conceptual model (model structure) and observation data. According to Atangana and Van Tonder (2014), parameter uncertainty can be defined as “uncertainty that arises in selecting values for parameters in the various models”. Parameters associated with ground water models include hydraulic conductivity, transmissivity, specific yield, storage coefficient and dispersivity. Since hydrogeological data from the field is always limited, parameter uncertainty is derived from unreasonable parameter division, the temporal and spatial variability and the scaling effect of parameters. Conceptual model (model structure) uncertainty is influenced by many factors, including the incorrect setting of model aquifers (location, type, number of layer, distribution, etc.), unreasonable estimation of ground water model’s boundary conditions and sources and sinks, and the approximation of special ground water processes.

Therefore, hydrogeological conditions are often simplified incorrectly by ground water conceptual model. Observation uncertainty stems from a very wide range, including the error caused by the stochastic distribution of the observed variable, indirect measurement error, the error of measuring device and human recording error, etc.

Due to uncertainties in modelling, every ground water model has limitations. Therefore, ground water models never uniquely represent the complexity of the real world. Groundwater models that represent the natural world have some level of uncertainty that must be evaluated and reported. In that respect, forecasting simulations for groundwater are similar to weather forecasts. Similar to weather forecasts, groundwater models should be qualified by specifying the nature and magnitude of uncertainty associated with a forecast (Mary *et al*., 2015).

1.2 PROBLEM STATEMENT

The Theis (1935) equation for groundwater flow in a confined aquifer is one of the fundamental solutions for the deterministic mathematical models of groundwater flow. The equation was derived based on certain assumptions such as: the aquifer is homogenous; has infinite aerial extent, isotropic and of uniform thickness; pumped at a constant discharge rate, etc. Based on the above assumptions, Theis simplified and ignored high order terms in the derivation of the groundwater flow equation for a confined aquifer. However, in reality, such is not the case as aquifers tend to be heterogenous, anisotropic, has finite aerial extent due to impermeable boundaries, and are pumped at different discharge rates, etc. This study will address such a problem by developing or rather modifying the groundwater flow equation for a confined aquifer. The derivation of the exact groundwater flow equation for a confined aquifer will not be limited by assumptions and no simplifications will be made to the equation. Following the new equation, a new numerical scheme for singular partial differential equations will also be developed. Theis and our solution will be compared using experimental data from different sites.

1.3 AIMS AND OBJECTIVES

The main aim of this research is developing the exact groundwater model within a confined aquifer.

Objectives include:

1.3.1 Deriving an exact groundwater flow equation in confined aquifer.

1.3.2 Prove that the above equation has unique solution.

1.3.3 Create and compare numerical simulations using the Melin transform, Adam Bashforth and Inverse Mellin transform to solve singular partial differential equation.

1.3.4 Solve the exact groundwater model within confined aquifers using the new numerical scheme.

1.3.5 To collect experimental data from different sites and compare them with Theis and our solution.

1.4 RESEARCH OUTLINE

The dissertation has seven chapters: chapter one provides a background of what modelling entails, uncertainties associated with modelling and the derivation of groundwater flow in a confined aquifer. Chapter two describes the literature review of uncertainties and sensitivity analysis in groundwater modelling. Chapter three presents analysis of exact groundwater model within a confined aquifer. Chapter three also shows prove that the new groundwater flow equation has unique solution and exists. Chapter four shows the creation of the new numerical scheme for singular partial differential equation. In addition, stability analysis using the von Neumann method is also provided in chapter four. Chapter five discusses the application of data in numerical modelling. Chapter five also incorporates interpolation of data and application of interpolation in groundwater. In chapter six, our solution was compared to Theis using experimental field data. Chapter six also shows numerical simulations of our model. Chapter seven entails the conclusion based on the whole research and recommendations are also discussed in this chapter.

1.5 RESEARCH FRAMEWORK

The following framework was used to achieve the main aim and objectives of this study:

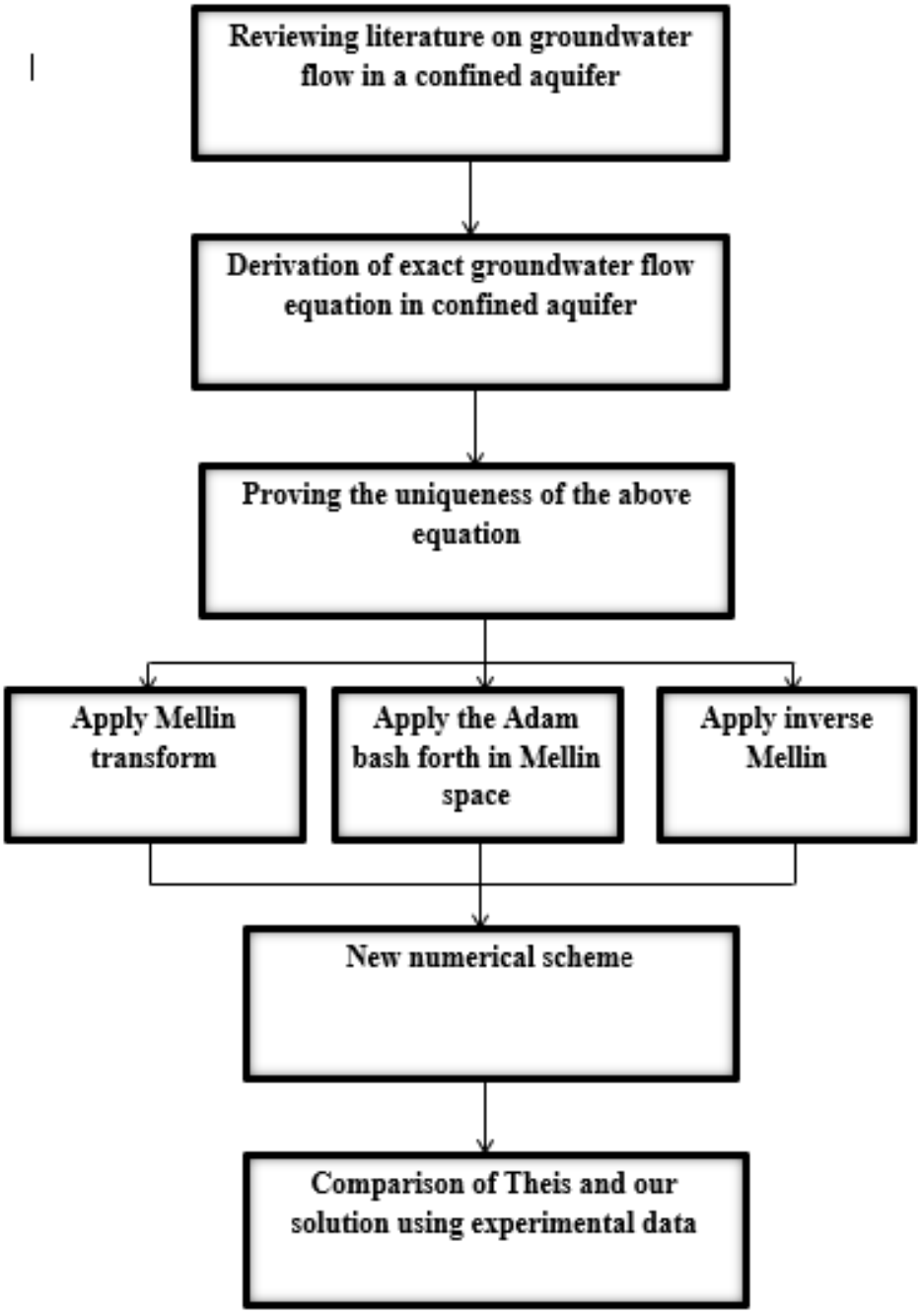

Figure 1: Research Framework followed in this study.

1.6 DERIVATION OF GROUND WATER FLOW IN CONFINED AQUIFER

The derivation of ground water flow in a confined aquifer starts from Darcy's law. Darcy's law is a simple proportional relationship between the instantaneous discharge rate through a porous medium, the viscosity of the fluid and the pressure drop over a given distance.

From Darcy's law, we get:

$$q = -K\frac{\partial h}{\partial r} \tag{1.2}$$

$$Q = -KA\frac{\partial h}{\partial l} \tag{1.3}$$

Where q is the Darcy flux (m/s), Q is the discharge (m^3/day), K is the hydraulic conductivity (m/day), $\frac{\partial h}{\partial l}$ is known as hydraulic gradient, A is the cross sectional of flow (m^2). The negative sign signifies that ground water flows in the direction of head loss.

Based on the principle continuity equation of flow, the difference between the rate of inflow and the rate of outflow from an annular cylinder is equal to the rate of change of volume of water within the cylinder.

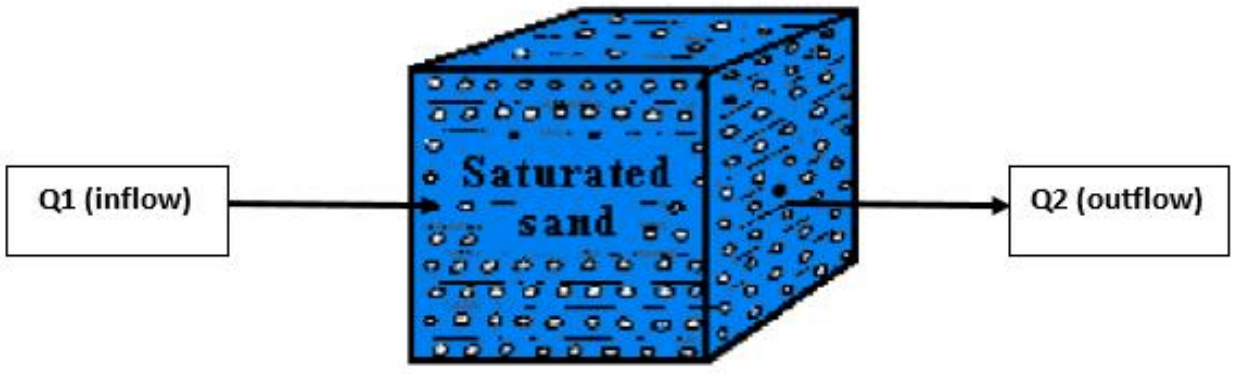

Figure 2: Diagram depicting Inflow and Outflow in a porous medium (Google/Images, 2017).

Thus,

$$Q_1 - Q_2 = \frac{\partial v}{\partial t} \tag{1.4}$$

Where Q_1 is the rate of inflow, Q_2 is the rate of outflow and $\frac{\partial v}{\partial t}$ is the rate of change of volume (V).

The slope of the hydraulic gradient line (i.e. the piezometric surface) at the inner surface is given as $\frac{\partial h}{\partial t}$, where h is the height of piezometric surface above the impermeable stratum. This means that the slope of the hydraulic gradient line at the outer surface is equal to,

$$\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2} dr \tag{1.5}$$

By Darcy's law.

$$Q = KIA$$

Substituting hydraulic gradient and area in the above equation, we get:

$$Q_1 = K\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2} dr\right].2\pi(r + dr)\ b$$

$$Q_2 = K\frac{\partial h}{\partial r}\ .(2\pi r)\ b \tag{1.6}$$

Based on the definition of storage coefficient (S), is the volume of water released per unit surface area per unit change in head normal to the surface. Therefore,

$$Change\ in\ volume = \partial V = S(2\pi r)\ dr.\partial h$$

$$\frac{\partial v}{\partial t} = S(2\pi r)\ dr\frac{\partial h}{\partial t} \tag{1.7}$$

By replacing equation (1.6) and (1.7) in equation (1.4), we get:

$$Kb\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2}\partial r\right].2\pi(r + \partial r) \tag{1.8}$$

$$-Kb\left[\frac{\partial h}{\partial r}\right].(2\pi r) = S(2\pi r)\,\partial r\frac{dh}{dt}$$

The above equation is thus divided by $Kb\ (2\pi r)\ dr$ throughout and higher order terms are neglected.

Thus,

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}.\frac{\partial h}{\partial r} = \frac{S}{Kb}.\frac{\partial h}{\partial t} \tag{1.9}$$

Since Transmissivity $(T)\ =\ Kb$, we substitute transmissivity for Kb,

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}.\frac{\partial h}{\partial r} = \frac{S}{T}.\frac{\partial h}{\partial t} \tag{1.10}$$

Where h is the head, r is radial distance from the well, s is storage coefficient, T is transmissivity and t is the time since the beginning of pumping. Above is the basic equation of unsteady flow towards the well.

1.7 DERIVATION OF EXACT SOLUTION OF GROUNDWATER FLOW MODEL IN CONFINED AQUIFER USING ANALYTICAL METHODS.

There are three different analytical methods for solving the new groundwater flow equation.

1.7.1 Method of Separation of Variable

According to Atangana and Ünlü (2016) separation of variables, also known as the Fourier method, is any of the several methods for solving ordinary and partial differential equations, in which algebra allows one to rewrite an equation so that each of two variables occurs on a different side of the equation. For a partial differential equation with two parameters, the method assumes that the solution is in form of:

$$h(r,t) = U(r)V(t) \tag{1.11}$$

The above equation is then replaced in the main equation, and two different equations are obtained with the inclusion of the eigen value.

This method shall be used to derive the solution of the new groundwater flow equation. Replacing equation (1.11) into equation (1.10), we get:

$$V(t)\frac{dU(r)}{dr} + V(t)\frac{d^2U(r)}{dr^2} = \frac{S}{T}dt\big(V(t)\big)U(r) \tag{1.12}$$

By rearrangement, we get the following equations:

$$\begin{cases} \dfrac{dU(r)}{dr} + \dfrac{d^2U(r)}{dr^2} = -\lambda^2 \\ \dfrac{S}{T}dt[v(t)] = -\lambda^2 v(t) \end{cases} \tag{1.13}$$

Here λ is known as eigen values. The first equation in the above can be solved using the Sumudu transform. The Sumudu transform of a function posits that $f\ (x)$ is defined as:

$$S\big(f(x)\big)(u) = \int_0^\infty \frac{1}{u}\exp\left[-\frac{x}{u}\right] f(x)\ dx \tag{1.14}$$

The following are useful properties of the Sumudu transform operator:

$$S\big(f(x)\big)(u) = \frac{F(u) - f(0)}{u}, \tag{1.15}$$

$$S\big(f''(x)\big)(u) = \frac{F(u) - f(0)}{u^2} - \frac{f(0)}{u}, \tag{1.16}$$

$$S\left[\frac{1}{x}f'(x)\right](u) = \frac{1}{u}\frac{dF(u)}{du}, \tag{1.17}$$

By applying on both sides of the equation using the above properties, we obtain the following expression:

$$\frac{1}{u}\frac{dU(u)}{du}\frac{U(u) - U(0)}{u^2} - \frac{U'(0)}{u} = \lambda^2 U(u). \tag{1.18}$$

Rearranging, and taking into account the boundary condition, we get:

$$u\frac{dU(u)}{du} + (1 + (\lambda u)^2)\ U(u) = 0. \tag{1.19}$$

Equation (1.20) can further be arranged as follows:

$$\frac{dU\,(u)}{U\,(u)} = \frac{(1+(\lambda u))^2}{u}\,du. \tag{1.20}$$

The exact solution of the above equation is as follows:

$$U(u) = \exp\left[-\int \frac{(1+(\lambda u)^2}{u}\right]. \tag{1.21}$$

Furthermore, applying the inverse Sumudu transform on both sides of equation (1.21) we get the following solution:

$$U(r) = J_0\,(\lambda^2 r). \tag{1.22}$$

The above expression is known as the Bessel function of the first kind and is defined as:

$$J_0[r] = \sum_{n=0}^{\infty} \frac{(-1)^k}{K!}\frac{1}{\Gamma(k+1)}\left(\frac{r}{2}\right)^{2k} \tag{1.23}$$

The second equation of Relation (15) that is:

$$\frac{S}{T}\frac{d}{dt}[V(t)] = -\lambda^2 V(t), \tag{1.24}$$

Has an exact solution:

$$V(t) = cexp\left[-\frac{T\lambda^2}{\alpha S}(t)\right]. \tag{1.25}$$

Thus, applying the procedure of separation of the variables, we get the exact solution of the new groundwater flow equation as:

$$h(r,t) = c\sum_{n-0}^{\infty} exp\left[-\frac{T\lambda_n}{\alpha S}(t)\right]J_0[\lambda_n r]. \tag{1.26}$$

Using the initial condition, we obtain the exact solution of the new groundwater equation to be:

$$h(r,t) = \frac{Q}{4\pi T}\sum_{n-0}^{\infty} exp\left[-\frac{T\lambda_n}{\alpha S}(t)\right]J_0[\lambda_n r]. \tag{1.27}$$

1.7.2 Laplace-Transform Method

The second analytical method for solving the new groundwater equation is the Laplace-transform method.

Let f be a function such that for any $0 < \beta \leq n$ the Laplace transform of $F(t)$ exists, then the Laplace-transform of f is defined as:

$$L_\beta(f))(s) = \int_0^\infty f\,(t)\exp[-st]dt. \tag{1.28}$$

Thus, applying the Laplace-transform on both sides of equation (1.10), we get:

$$\frac{\partial H(r,s)}{r\partial r} + \frac{\partial^2 H(r,s)}{\partial r^2} = \frac{S}{T}\big(sH(r,s) - h(r,0)\big). \tag{1.29}$$

By applying the Laplace-transform on both sides, we get:

$$u\frac{dH(r,s)}{du} + u^2H(r,s) - u^2H(0,s) - \lambda^2H(u,s) = 0. \tag{1.30}$$

With:

$$\lambda^2 = s\frac{S}{T}. \tag{1.31}$$

Applying the boundary condition together with the initial condition, we get the following:

$$u\frac{dH(u,s)}{du} + (u^2 - \lambda^2)H(u,s) = 0. \tag{1.32}$$

The exact solution of the above equation is given as:

$$U(r,s) = J_0\left(s\frac{S}{T}u\right). \tag{1.33}$$

Thus, applying the inverse Laplace twice for s and u, we get the exact solution as:

$$h(r,t) = c\int_u^\infty \frac{1}{t}\exp\left[-\frac{T\lambda^2}{\alpha S}(t)\right]dt, \tag{1.34}$$

By applying the initial condition again, we get the following exact solution of the new groundwater equation within a confined aquifer:

$$h(r,t) = \frac{Q}{4\pi T}\int_{u}^{\infty}\frac{1}{t}\exp\left[-\frac{T\lambda^2}{\alpha S}(t)\right]dt = \frac{Q}{4\pi T}W_{\beta}(u) \tag{1.35}$$

$$u = \frac{r^2 S}{4Tt}h(r,t) = \frac{c}{t-t_0}\exp[-u_{\beta 0}]. \tag{1.36}$$

The following integral will be referred to as beta-exponential integral:

$$\int_{0}^{\infty}\frac{1}{t}\exp\left[-\frac{T\lambda^2}{\alpha S}(t)\right]dt. \tag{1.37}$$

1.7.3 Alternative Method

The third method used was an alternative method which was used to derive the exact solution of the new groundwater flow equation. This method is often used for some classes of parabolic partial differential equation. This method used the concept of reduction of dimension; in particular, the method used the Boltzmann transformation (Atangana and Ünlü, 2016). In this method, defined for an arbitrary $t_0 < t$ by equation:

$$u_0 = \frac{Sr^2}{4T(t-t_0)}. \tag{1.38}$$

However, in the case of the new groundwater flow equation, the above equation cannot be used, and to extend this method to the scope of beta-partial differential equation, Atangana and Ünlü (2016) proposed the following transformation:

$$u_{\beta 0} = \frac{Sr^2}{4T[(t-t_0)]}. \tag{1.39}$$

Now, considering the following function:

$$h(r,t) = \frac{c}{t-t_0}\exp\left[-u_{\beta 0}\right]. \tag{1.40}$$

With c being any arbitrary constant. If we assume that r_b is the ratio of the borehole from which the groundwater is being taken out from the aquifer, thus, the total volume of the water withdrawn from the aquifer is provided by:

$$Q_0 \Delta t_0 = 4\pi cT. \tag{1.41}$$

Here:

$$h(r,t) = \frac{c}{t - t_0} \exp\left[-u_{\beta 0}\right], \tag{1.42}$$

Is the drawdown which will be experimental at a detachment, r from the pumping well after the time space of Δt_0. Now, γ, assume that the above formula is continual m-times, meaning that water is being removed for a very short period of time, Δt_k, at consecutives times. $t_{k+1} = t_k + \Delta t_k$, $(k = 0, 1, 2, \dots, m)$. In this instance, since the new groundwater flow equation is linear, the total drawdown at any time $t > t_k$ is given by:

$$h(r,t) = \frac{1}{4\pi T} \sum_{k=0}^{n} \frac{\Delta t_k Q_k}{t - t_k} \exp\left[-u_{\beta 0}\right]. \tag{1.43}$$

In the above equation, the summation can be transformed into an integral if $\Delta t \to 0$, then equation (1.44) becomes:

$$h(r,t) = \frac{1}{4\pi T} \int_{t_0}^{t} Q(x) \frac{\exp[-u_{\beta 0}]}{t - x} dx \tag{1.44}$$

A particular important solution which arises when t_0 is considered at the origin zero and at the point where the discharge rate is independent of time, then equation (1.43) becomes:

$$h(r,t) = \frac{Q}{4\pi T} \int_{u}^{\infty} \frac{1}{t} \exp\left[-\frac{T\lambda^2}{\alpha S}(t)\right] dt = \frac{Q}{4\pi T} W_{\beta}(u). \tag{1.45}$$

CHAPTER 2: LITERATURE REVIEW OF UNCERTAINTIES AND SENSITIVITY ANALYSES

2.1 UNCERTAINTIES OF GROUNDWATER MODEL

The most direct method for assessing uncertainties is to derive the statistical information of output directly. However, the direct method is infeasible in practical application. This is due to challenges in mathematics and numerical solution when deriving statistical result. The other challenge is that the statistical properties on the system structure and input are mostly unknown. This chapter discusses the various methods and techniques to analyze uncertainties of model parameters, conceptual model and observation data.

2.2 UNCERTAINTY ANALYSIS OF GROUNDWATER MODEL PARAMETERS

Choosing appropriate model parameters to use on the model is the first step or challenge that has to be faced. The choice of model parameters will have a great influence on the simulated results. The parameters of a groundwater model such as hydraulic conductivity, are always uncertain because of measurement error, heterogeneity, and scaling issues. In the past few decades, there has been developments of various methods and techniques for assessing the impact of input parameter uncertainty on model predictions.

According to JiChun and XianKui (2013), the most popular and feasible methods for parametric uncertainty are Generalized Likelihood Uncertainty Estimation (GLUE), Markov Chain Monte Carlo (MCMC), Bayesian Recursive Estimation (BARE), etc.

2.2.1 Generalized Likelihood Uncertainty Estimation (GLUE)

GLUE is a Monte Carlo Simulation technique based on the equifinality (Beven and Binley, 1992; Beven and Freer, 2001). It rejects the idea of a single correct representation of the system in favor of many acceptable or behavioral system representations that should be considered in the evaluation of uncertainty associated with predictions (Beven, 2006).

For each simulator sampled from a prior set of possible system representation a likelihood measure is calculated that reflects the ability of the simulator to simulate the system responses. Simulations that perform below a rejection criterion are discarded from the further analyses and the likelihood measures of retained simulators are rescaled so as to render the cumulative likelihood equal to one. Ensemble predictions are based on the predictions of the retained set of simulators, weighted by their respected rescaled likelihood.

The likelihood or “goodness of fit” used in GLUE are a measure of the ability (performance) of a simulator to reproduce a given set of observed system responses. Therefore, they represent an expression of belief in the predictions of that particular simulator rather than a formal definition of probability being the correct representation of the system (Binley and Beven, 2003). GLUE has the advantage of simple structure, easy operation and wide applicability. GLUE has been widely used for many purposes, such as precipitation-runoff model, distributed basin hydrological model, soil erosion model, groundwater model, unsaturated zone model and flood model. GLUE has some shortcomings. Due to the ineffective sampling technique, this method requires a large number of simulations to obtain the convergence of Monte Carlo simulation. Furthermore, for complex and high-dimensional uncertainty issues, it is likely to generate unreliable and inconsistent result (JiChun and XianKui, 2013).

2.2.2 Markov Chain Monte Carlo (MCMC)

Markov Chain Monte Carlo (MCMC) is a dynamic sampling technique. By constructing a Markov Chain with stable density distribution, the probability distribution space of target function is sufficiently searched in the process of evolving Markov Chain. The searching process is constructed by two functions which are proposal and acceptance functions. Proposal function (or proposal distribution) is used for generating alternative sample of parameter set, and whether the parameter sample is accepted or rejected depends on acceptance function (or transition function). Sampling algorithm is the core of MCMC, which determines the sampling efficiency and reliability of uncertainties analysis (JiChun and XianKui, 2013).

MCMC methods use two sampling techniques, namely single-chain and multi-chain techniques. Single-chain techniques was developed in early MCMC methods. (Metropolis *et al.,* 1953) proposed the Metropolis algorithm to simulate energy levels of atoms in crystal structure. Based on Metropolis algorithm, (Hastings *et al.,* 1970) developed Metropolis-Hastings (M-H) algorithm which is able to make use of any form of transition function, and meet the requirement of detailed balance. (Haario *et al.,* 1999) developed an adaptive proposal distribution (AP) algorithm, AP is operated by a normal distribution of which the mean and variance are calculated by retained samples. Based on AP algorithm, (Haario *et al.,* 2001) developed an Adaptive Metropolis (AM) algorithm, with respect to AP, AM is superior in updating the mean and covariance of proposal distribution by using previous sampling information based on a regression formula.

(Vrugt *et al.,* 2003) developed a multi chain evolving algorithm, Shuffled Complex Evolution Metropolis algorithm (SCEM) which assembles the advantages of M-H algorithm, controlling random search, competition evolution and shuffled complex evolution. The convergence rate is improved by adopting multiple parallel Markov chains, and exchanging searching information between chains. (Braak *et al.,* 2006) reported a genetic algorithm based differential evolution Markov Chain (DE-MC). This is a multi-chain parallel evolution technique by combining MCMC and differential evolution method. Based on DE-MC, (Vrugt *et al.,* 2009) proposed a differential evolution adaptive Metropolis algorithm (DREAM). This method generates a proposal sample based on the difference of one (or several) couple of parameter samples. In addition, the adopted strategies of DREAM include sampling from a group of updated random subspaces, estimating the probability distribution of the cross probabilities of random subspaces. Therefore, the convergence rate of DREAM is improved significantly.

MCMC method is superior in strong flexibility, high reliability in various environmental models uncertainty analysis. MCMC method has a good performance on complex uncertainty issues which include high nonlinear, high dimensional and multimodal probability distribution. MCMC method is inferior in huge computing time-consuming requirement. In addition, MCMC method is restricted in the application of parallel computing techniques because of its logic computing characteristics.

2.2.3 Bayesian Recursive Estimation (BARE)

Bayesian Recursive Estimation (BARE) requires only an initial guess of the region of the parameter estimates to be specified before the model can be used to begin the generation of one-step ahead (and multiple-step-ahead) predictions. These predictions are described in terms of the probabilities associated with different output values (or can be summarized in terms of a “most likely” prediction and a “Bayesian confidence interval”). The uncertainty associated with the prediction will be relatively large in the beginning. A recursive procedure is used to update (reduce) the uncertainty associated with the parameter estimates as successive input-output measurement data are assimilated. The reduced parameter uncertainty results in smaller prediction uncertainties (Thiemann *et al.,* 2001).

2.3 UNCERTAINTY ANALYSES OF GROUNDWATER CONCEPTUAL MODEL

Conceptual models have many uncertainties due to both the scarcity of data and subjectivity of many modelling decisions. Modelers are forced to make simplistic assumptions of reality. Model errors are introduced in, for example, the parameterization, discretization, parameter zonation and boundary conditions selected. Uncertainties in the conceptual model have been recognized as a main source of uncertainty in model prediction (Usunoff *et al.,* 1992; Neumann and Wierenga, 2003; Hojberg and Refsgaard, 2005). Three types of model uncertainties can be defined: conceptual model uncertainty, mathematical model uncertainty, and computer code uncertainty (Zio and Apostolakis, 1996). In general, the sources of model uncertainty can be further classified as follows:

2.3.1 Model Structure

The uncertainty in model structure and mathematical equation is referred to as conceptual error (Hua lei and Schilling, 1996). This type of uncertainty arises from the simplification made in the mathematical computation in the model structure. Model structure is the reason of different solution and output between one model and another (Baalousha, 2003).

2.3.2 Model Concept

Every model concept arises from assumptions made about the aquifer properties. These assumptions do not always take into account the complexities of the aquifer (heterogeneity) and as such result in another type of uncertainty. Boundary and initial conditions also play an important role in the modelling process and affects the output of the model.

2.3.3 Model Resolution

In terms of accuracy, more finer elements in the model domain result in more accurate solution. On the other hand, as the number of elements increases, the computation time increases as well. For this reason, the selection of mesh size is important in terms of accuracy and can result in uncertainty if the mesh is coarse (Baalousha, 2003).

However, the existing approaches for coping with conceptual model uncertainties are neglected, and uncertainties analyses are performed considering only parameter uncertainty and using only a single conceptual model. As the development of uncertainty analysis in groundwater conceptual model, the multi-model method has become an important theory in treating groundwater modelling uncertainty. The groundwater system is represented by a set of conceptual models which are weighted by their corresponding performance on reproducing the groundwater system (Refsgaard *et al.,* 2007). The behavior of unknown groundwater system is described by the combination of outputs of alternative models. In general, multi model analysis includes the following steps: (1) constructing a group of plausible conceptual models based on prior information; (2) calibrating these alternative conceptual models by obtained conditioning data; (3) weighting or ranking these conceptual models by using a criterion; (4) removing these models with significantly unreasonable performances; (5) ensemble prediction by combining the weighted predictions of retained conceptual models.

Poeter and Anderson (2005) proposed a Kullback-Liebler information based multi-model theory, this method can evaluate the weight of alternative models, but the prior information cannot be formally incorporated into assembled predictions. (Refsgaard *et al.,* 2006) developed a pedigree analysis method to assess conceptual model uncertainty, this method is able to integrate various kinds of prior knowledge. However, each part of predictive uncertainty cannot be delineated quantitatively. Bayesian Model Averaging method is firstly proposed by (Drapper, 1995; Kass *et al.,* 1995), this method infers the posterior probabilities of alternative conceptual models based on Bayesian inference, and each part of predictive uncertainty can be described separately. The formula of BMA is given as:

$$P(\Delta \mid Z) = \sum_{k=1}^{d} P\,(\Delta|Z, M_k)\; P(M_k \mid Z) \tag{2.1}$$

Where Δ denotes a predictive variable, $p(\Delta \mid Z)$ is the ensemble probability of Δ, and $P(\Delta|Z, M_k)$ represents the probability of Δ given observation Z and model M_k. $p(M_k|Z)$ is the posterior probability of model M_k, which can be computed using Bayesian theorem;

$$P(M_k \mid Z) = \frac{P(Z \mid M_k)\; P\,(M_k)}{\sum_{i=1}^{k} P\,(Z \mid M_i)\; P(M_i)} \tag{2.2}$$

Where $p(M_k)$ denotes the prior probability of model M_k, $p\,(Z|M_k)$ is the intergrated likelihood measure of conceptual model M_k.

Conceptual model's posterior probability is obtained by combining conceptual model's prior probability and integrated likelihood value $p(Z|M_k)$ which indicates the performance on reproducing groundwater observations (Kass *et al.,* 1995; Rojas *et al.* 2010). Moreover, the variance of groundwater model's prediction is divided into within-model and between-model variances which represent the uncertainties of model parameter and structure respectively (Rojas *et al.,* 2008; Ye *et al.,* 2010).

BMA methods can be divided into two broad categories; the Monte Carlo based BMA method (MC-BMA) and the information criteria (or model selection criteria) based BMA method (IC-BMA). Kullback-Liebler (K-L) information is the base of model selection theory.

When information criteria are used for selecting models, each conceptual model will obtain a K-L value which represents the loss of information as the real groundwater system is represented by this model (Refsgaard e*t al.,* 2006). Therefore, a series model selection criterion is developed for estimating K-L value, e.g. Akaike Information Criterion (AIC), second-order-bias-corrected AIC (AIC_c), Bayesian Information Criterion (BIC), and Kashyap Information Criterion (KIC), (Neuman and Wirenga, 2003; Burnham and Anderson, 2005).

IC-BMA is the main idea for current multi-model averaging methods. Neuman and Wirenga (2003) proposed a suit of strategies for constructing and selecting conceptual models, assembling model's outputs and making optimum prediction, which is lack of formality. Neuman (2003) proposed a KIC based Maximum Likelihood Bayesian Modelling Average (MLBMA) to overcome this defect. MLBMA can integrate the information on field conditions and observations, and the final outcome depends on the combination of model outputs and prior information.

The software Multi-Model Analysis (MMA) is a convenient and efficient tool for conceptual model's uncertainty analysis. MC-BMA method calculates conceptual models integrated likelihood value $p(Z|M_k)$ by Monte Carlo simulation which is applied to inverse model's parameter space. (Rojas *et al.,* 2008) firstly proposed GLUE based BMA method, for which GLUE is used to estimate conceptual models integrated likelihood value. In addition, (Rojas *et al.,* 2010) pointed that for IC-BMA method, the application of information criteria includes a step of model calibration. Thus, model structures deviation could be compensated by model calibration, which will cause statistical bias of conceptual model's posterior probability. By contrast, MC-BMA determines posterior weight based on the likelihood distribution of corresponding conceptual model and its prior probability. Therefore, MC-BMA prevents multi-model average prediction from the erosion of biased parameter estimation.

Furthermore, (Raftery *et al.,* 2005) proposed an Expectation Maximization (EM) method to solve the weight and variance of conceptual models iteratively. EM-BMA assumes that model's prediction follows normal distribution, and it is hard to assure that EM algorithm convergences to global optimum's weight and variance.

2.4 UNCERTAINTY ANALYSIS OF GROUNDWATER OBSERVATION DATA

Observation errors are produced in the processes of measuring, collecting, recording, storing and importing data. They include system and random errors. When groundwater model is calibrated and verified based on a group of biased observation data, the uncertainties related to model output, parameter inversion, output prediction, etc., are regarded as observation error. Observation error is always merged with other sources, such as model parameter and structure uncertainties, to affect model output simultaneously. Uncertainty analysis of groundwater observation data has not been given enough attention in comparison with model parameter and conceptual model uncertainties. Observation data has always been assumed to be accurate, or given a simplified error structure (Post *et al.,* 2008; Renard *et al.,* 2009). Groundwater model observation uncertainty is assessed combined with the uncertainty analysis of model parameter and or structure. Furthermore, groundwater is an open system, the simulation errors stem from multiple sources, and data scarcity is the special factor which enhances the uncertainty of groundwater numerical simulation. Therefore, the residuals will often have a complicated structure that is hard to delineate or interpret (JiChun and XianKui, 2013).

Presently, observation uncertainty is usually assessed by comprehensive evaluation methods. The common used methods include Bayesian Forecasting System (BFS), integrated Bayesian uncertainty estimator (IBUNE), Bayesian total error analysis (BATEA), and data fusion method (Krzysztofo, 1999; Ajami *et al.,* 2007; Nowak *et al.,* 2010). (Troldborg et al., 2010) proposed an assembled method which combines Bayesian model averaging, Bayesian geostatistics method and Kalman ensemble generator to account for conceptual model and measurement uncertainties. In addition, the observation error is assumed to be normal and independent with zero mean and a fixed covariance matrix. (Refsgaard et al., 2010) evaluated the predictive uncertainty of a conceptual rainfall-runoff model based on BATEA. Furthermore, the total uncertainty was divided into input and structure uncertainties, and they were described and assessed quantitatively.

(Renard *et al.,* 2009) made a comparison between IBUNE and BATEA, and drew a conclusion that these two methods are both constructed based on the hierarchical generalized processing of input uncertainty. Moreover, for the first type of IBUNE, the likelihood function and posterior distribution are predictive variables stochastic functions, which is inconsistent with the standard essential function. In addition, the second type of IBUNE is inferior in sampling efficiency and convergence rate (JiChun and XianKui, 2013).

2.5 SENSITIVITY ANALYSIS OF GROUNDWATER MODEL

Sensitivity analysis is “the study of how uncertainty in the outputs of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input” (Saltelli *et al.,* 2004). Uncertainty analysis focuses rather on quantifying uncertainty in model output. Ideally, uncertainty analyses and sensitivity analyses should be run in tandem with uncertainty analyses preceding. Sensitivity analysis can serve a number of useful purposes in the economy of modelling. It can surprise the analyst, uncover technical regions in the space of the inputs, establish priorities for research, simplify models and defend against falsifications of the analysis.

According to Reilly and Harbaugh (2004) Sensitivity analysis is the evaluation of model input parameters to see how much they affect model outputs, which are heads and flows. The relative effect of the parameters helps to provide fundamental understanding of the simulated system. Sensitivity analysis also is inherently part of model calibration. The most sensitive parameters will be the most important parameters for causing the model to match observed values. For example, an area in which the model is insensitive to hydraulic conductivity generally indicates an area where there is relatively little water flowing.

If the model is being calibrated, then changing the value of hydraulic conductivity in this area will not help much in causing the model to match observations. The calibration will not provide much certainty about the value of the parameter, but the uncertainty will not matter provided the model is not used in situations where large amounts of water will flow in that area. Such a model, however, would probably not be suitable for evaluation of recharge or withdrawal in this area because the amount of flow in the area would be much greater than it was when the model was calibrated, and the uncertainty from the calibration would be unacceptable.

Sensitivity analysis can be conducted manually or automatically. In the manual approach, multiple model simulations are made in which ideally a single parameter is adjusted by an arbitrary amount. The changes to the model output for all of the parameter changes may be displayed in tables or graphs for evaluation. The automatic approach directly computes parameter sensitivity, which is the change in head or flow divided by the change in a parameter. Automatic sensitivity analysis is inherently part of automatic parameter adjustment for model calibration. The automatic parameter adjustment algorithm uses parameter sensitivity to compute the parameter values that cause the model to best match observed heads and flows (Reilly and Harbaugh, 2004).

2.5.1 Probabilistic Sensitivity Analysis

Mathematical models are built to simulate complex real-world phenomena. Such models are typically implemented in large computer programs and are also very complex, such that the way that the model responds to changes in its inputs is not transparent. Sensitivity analysis is concerned with understanding how changes in the model inputs influence the outputs. This may be motivated simply by a wish to understand the implications of a complex model but often arises because there is uncertainty about the true values of the inputs that should be used for a particular application. A broad range of measures have been advocated in the literature to quantify and describe the sensitivity of a models output to variation in its inputs. In practice, the most commonly measures are those that are based on formulating uncertainty in the model inputs by a joint probability distribution and then analyzing the induced uncertainty in outputs, an approach which is known as probabilistic sensitivity analysis (Oakley and O'Hagan, 2004).

2.5.1.1 Main Effects and Interactions

Sensitivity analysis methods can be seen in terms of a decomposition of the function $\eta(.)$ into main effects and interactions:

$$y = \eta(x) = E(Y) + \sum_{i=1}^{d} Z_i\ (X_i) + \sum_{i<j} Z_i\ Z_i, j, (X_i, j)$$

$$\sum_{i<j<k} Z_i\ , j, K(X_i, j, K) + \cdots + Z_{1,2,\ldots,} d(X) \tag{2.3}$$

$$Z_i(X_i) = E(Y|X_i) - E(Y), \tag{2.4}$$

$$Z_{i,j}(X_i) = E\left(Y\middle|X_{i,j}\right) - Z_i(X_i) - Z_j\left(X_j\right) - E(Y), \tag{2.5}$$

$$Z_{i,j,k}\left(X_{i,j,k}\right) = E\left(Y\middle|X_{i,j,k}\right) - Z_{i,j}\left(X_{i,j}\right) - Z_{i,k}\left(X_{i,k}\right)$$

$$Z_{j,k}\left(X_{j,k}\right) - Z_i(X_i) - Z_j\left(X_j\right) - Z_k(X_k) - E(Y), \tag{2.6}$$

And so on. Refer $Z_i(X_i)$ as the main effect of X_i, to $Z_{i,j}(X_{i,j})$ as the first order interaction between X_i and X_j, and so on.

The definitions of these terms depend on the distribution G of the uncertain inputs. Considering, for instance, the very simple model $\eta\ (X_1, X_2) = X_1$. We have $E(Y) = E(X_1)$ and $Z_1(X_1) = X_1 - E(X_1)$. If G is such that X_1 and X_2 are independent then $Z_2(X_2) = 0$ and $Z_{12}(X_1, X_2) = 0$. In this case, the representation reflects the structure of the model itself, comprising a linear effect of X_1 with no X_2-effect and no interaction. If, X_1 and X_2 are not independent, we get $Z_2(X_2) = E(X_1|X_2) - E(X_1) = -Z_{12}(X_1, X_2)$, which will not in general be 0. Computing and plotting the main effects and first order interactions is a powerful visual tool for examining how the model output responds to each individual input, and how these inputs interact in their influence on Y.

2.5.1.2 Variance Based Methods

Variance based methods of probabilistic sensitivity analysis quantify the sensitivity of the output Y to the model inputs in terms of a reduction in the variance of Y. Two principal measures of the sensitivity of Y to an individual X_i are proposed.

The first principle was proposed by (Saltelli *et al.,* 2000), is

$$V_i = var\,\{E(Y|X_i)\} \tag{2.7}$$

The motivation for this measure is that it is the expected amount by which the uncertainty in Y will be reduced if we learn the true value of X_i. Thus, if we were to learn X_i, then the uncertainty about Y would become Var $(Y|X_i)$, a difference of Var $(Y) - E\,\{Var(Y|X_i)\} = V_i$, by a well-known identity. Although Var$(Y) - Var(Y|X_i)$ can be negative for some X_i, its expectation V_i is always positive, so this is the expected reduction in uncertainty, due to observing X_i. $V_i = Var\,\{Z_i\,(X_i)\}$ and so is based on the main effect of X_i.

The second measure, first proposed by Homma and Saltelli (1996), is

$$V_{Ti} = Var(Y) - Var\{E(Y\ |X - i)\}, \tag{2.8}$$

Which is the remaining uncertainty in Y that is unexplained after we have learnt everything except X_i. Both measures are converted into scale invariant measures by dividing by Var (y):

$$S_i = \frac{V_i}{Var\,(Y)} \tag{2.9}$$

$$S_{Ti} = \frac{V_{Ti}}{Var(Y)} = 1 - S - i \tag{2.10}$$

Thus, Si may be referred to as the main effect index of X_i, and S_{Ti} is known as the total effect index of X_i. The relative importance of each input in driving the uncertainty in Y is then gauged by comparing their indices. As well as indicating the relative importance of an individual X_i in driving the uncertainty in Y. Equation (2) can be seen as indicating where to direct effort in future to reduce that uncertainty. In practice, it is rarely possible to learn the true value of any of the uncertain inputs exactly; nor is the cost of gaining more information likely to be the same for each input.

Nevertheless, the analysis does suggest where there is the greatest potential for reducing uncertainty through new research. It is not believed that there is any comparable interpretation of S_{Ti} in terms of guiding research effort. It does not follow that the two inputs with the largest main effect variances will be the best two inputs to observe.

We would need to calculate;

$$V_{i,j} = Var\left\{E\left(Y\middle|X_{i,j}\right)\right\} = Var\left\{Z_i\left(X_i\right) + Z_j\left(X_j\right) + Z_{ij}\left(X_{i,j}\right)\right\} \quad (2.11)$$

For all i and j, since this is the part of Var (Y) that is removed on average when we learn both X_i and X_j. The search for the most informative combinations of input is considered further by (Saltelli and Tarantola, 2002). In general, $V_p = Var\left\{E\left(Y\middle|X_p\right)\right\}$ is the expected reduction in variance that is achieved when we learn X_p.

2.6 LIMITATIONS IN PERFORMING UNCERTAINTY ANALYSIS

The main limitation in performing comprehensive uncertainty analyses of Groundwater models is the associated cost and effort. The computer resources required for uncertainty propagation using conventional methods can sometimes be prohibitively expensive. Further, the incorporation of uncertainty associated with structural and formulation aspects of the models requires significant effort. Finally, the data needs for characterizing input uncertainties are often substantial. Conventional methods for uncertainty propagation typically require several model runs that sample various combinations of input values. The number of model runs can sometimes be very large, i.e., of the order of many thousands, resulting in substantial computational demands.

On the other hand, in order to estimate the uncertainties associated with model formulation, several different models, each corresponding to a different formulation of the mathematical problem corresponding to the original physical system, have to be developed. The model results corresponding to all the possible combinations give an estimate of the range of the associated model uncertainty. Development and application of several alternative computational models can require substantial time and effort. Thus, the costs associated with uncertainty analysis may sometimes be prohibitively high, necessitating a large number of model simulations and/or the development of several alternative models.

2.7 LIMITS OF SENSITIVITY ANALYSIS

It is important, however, to recognize that the sensitivity of the parameter in the equation is what is being determined, not the sensitivity of the parameter in nature. Therefore, if the model is wrong or if it's a poor representation of reality, determining the sensitivity of an individual parameter in the model is a meaningless pursuit. Sensitivity analysis relies on assumptions (Saltelli, 2006).

CHAPTER 3: ANALYSIS OF EXACT GROUNDWATER MODEL WITHIN A CONFINED AQUIFER.

This chapter aims at deriving an exact solution for groundwater flow in a confined aquifer, proving that the equation exists and has unique solution. Numerical simulations will also be created and compared using the Melin transform and Inverse Mellin transform to solve singular partial differential equation. The derivation of the exact analytical solution of this equation will be shown. As mentioned in the previous sections of the last chapters, every groundwater flow in a confined aquifer starts from Darcy's law. The derivation of this problem is under the Theis conditions of groundwater flowing within a confined aquifer.

From Darcy's law, we get:

$$q = -K\frac{\partial h}{\partial r} \tag{3.1}$$

$$Q = -KA\frac{\partial h}{\partial r} \tag{3.2}$$

Where q is the Darcy flux (m/s), Q is the discharge (m^3/day), K is the hydraulic conductivity (m/day), $\frac{\partial h}{\partial t}$ is known as hydraulic gradient, A is the cross sectional of flow (m^2). The negative sign signifies that ground water flows in the direction of head loss.

Based on the principle equation of flow, we get that the water flowing into the porous medium minus the water flowing out of the porous medium is equal to the change in volume inside the porous medium with respect to time. To achieve this, we set up an equation for the head based upon the volume conservation in an annulus of thickness Δr with radial inflow and outflow. The choice of this radial flow is based on the fact that, the water enters the borehole symmetrically around the drilled borehole, which has cylindrical form. Mathematically, this can be represented as:

$$Q_1 - Q_2 = \frac{\partial v}{\partial t} \tag{3.3}$$

Where Q_1 is the rate of inflow, Q_2 is the rate of outflow and $\frac{\partial V}{\partial t}$ is the rate of change of volume (V).

Thus,

$$Q_1 = K\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2}\Delta r\right].2\pi(r+\Delta r)\ b \tag{3.4}$$

$$Q_2 = K\frac{\partial h}{\partial r}.(2\pi r)\ b$$

Based on the definition of storage coefficient (S), is the volume of water released per unit surface area per unit change in head normal to the surface.

Therefore,

$$Change\ in\ volume = \partial V = S(2\pi r)\ \Delta r.\partial h$$

Therefore,

$$\frac{\partial v}{\partial t} = S(2\pi r)\frac{\partial h}{\partial t}\ \Delta r \tag{3.5}$$

The area $(2\pi r)\,\Delta r$ in equation (3.5), which is the area of a cross-section through the annulus, suggested that there is flow normal to that area along the length of the annulus. By replacing equation (3.4) and (3.5) in equation (3.3), we get:

$$Kb\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2}dr\right].2\pi(r+dr)$$

$$-Kb\left[\frac{\partial h}{\partial r}\right].(2\pi r) = S(2\pi r)\ \Delta r\frac{\partial h}{\partial t} \tag{3.6}$$

By dividing the above equation with 2π, we get:

$$Kb\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2}dr\right].(r+\Delta r) \tag{3.7}$$

$$-Kb\left[\frac{\partial h}{\partial r}\right].r = S(r\Delta r)\frac{\partial h}{\partial t}$$

The above equation can be divided by rdr throughout, we get:

$$Kb\left[\frac{\partial h}{\partial r} + \frac{\partial^2 h}{\partial r^2}dr\right]\frac{r+\Delta r}{r\Delta r} - Kb\left[\frac{\partial h}{\Delta r\partial r}\right] = S\frac{\partial h}{\partial t} \tag{3.8}$$

Rearranging the above equation gives us:

$$Kb\left[\frac{\partial h}{\partial r}+\frac{r+\Delta r}{r\Delta r}+\frac{\partial^2 h}{\partial r^2}.\frac{\Delta r(r+\Delta r)}{r\Delta r}\right] \tag{3.9}$$

$$-Kb\left[\frac{\partial h}{\partial r\Delta r}\right]=S\frac{\partial h}{\partial t}$$

$$Kb\left[\frac{\partial h}{\partial r}.\frac{r}{r\Delta r}+\frac{\partial h}{\partial r}.\frac{\Delta r}{r\Delta r}+\frac{\partial^2 h}{\partial r^2}.\frac{r\Delta r}{r\Delta r}+\frac{\partial^2 h}{\partial r^2}.\frac{(\Delta r)^2}{r\Delta r}\right] \tag{3.10}$$

$$-Kb\left[\frac{\partial h}{\Delta r\partial r}\right]=S\frac{\partial h}{\partial t}$$

$$Kb\left[\frac{\partial h}{\Delta r\partial r}+\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}+\frac{\partial^2 h}{\partial r^2}.\frac{\Delta r}{r}\right] \tag{3.11}$$

$$-Kb\left[\frac{\partial h}{\Delta r\partial r}\right]=S\frac{\partial h}{\partial t}$$

Since Transmissivity $(T)=Kb$ we substitute transmissivity for Kb,

$$T\left[\frac{\partial h}{\Delta r\partial r}+\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}+\frac{\partial^2 h}{\partial r^2}.\frac{\Delta r}{r}\right]-T\left[\frac{\partial h}{\Delta r\partial r}\right]=S\frac{\partial h}{\partial t}$$

By dividing the above equation with T, we get:

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\left[\frac{\partial h}{\Delta r\partial r}+\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}+\frac{\partial^2 h}{\partial r^2}.\frac{\Delta r}{r}-\frac{\partial h}{\partial r\Delta r}\right] \tag{3.12}$$

Therefore,

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}\left[1+\frac{\Delta r}{r}\right] \tag{3.13}$$

Thus, above is the exact solution of the groundwater flow equation in a confined aquifer.

We now introduce a small perturbation term $\Delta r=scaling\ constant$.

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}\left[1+\frac{\Delta r}{r}\right] \tag{3.14}$$

Indeed, from equation (3.12) to equation (3.14) if one takes the limit as Δr tends to zero, one will recover the Theis groundwater flow model. The physical problem under investigation here is that of flow in an annulus of finite thickness. We now have to prove that the above equation has a unique solution. To determine if the above equation has a unique solution, we first have to prove that this operator is well defined and is also a contraction. For the operator to be a contraction, K (constant) must be less than 1. Thereafter, we must prove that the operator satisfies the Lipschitz condition. If the above conditions are satisfied, then this operator has a unique solution.

The above equation is divided by $\frac{S}{T}$, thus:

$$\frac{\partial h(r,t)}{\partial t} = \frac{T}{S}.\frac{\partial h}{r\partial r} + \frac{T}{s}.\frac{\partial^2 h}{\partial r^2}\left[1 + \frac{\Delta r}{r}\right] \tag{3.15}$$

The above equation is then reduced to:

$$\frac{\partial h(r,t)}{\partial t} = \frac{\partial h}{\partial r}a(r) + \frac{\partial^2 h}{\partial r^2}b(r) \tag{3.16}$$

$$\frac{\partial h}{\partial t} = f(h,t) \tag{3.17}$$

Where,

$$a(r) = \frac{T}{S}\frac{1}{r}$$

$$b(r) = \frac{T}{S}\left[1 + \frac{\Delta r}{r}\right]$$

Therefore,

$$f(h,t) = \frac{\partial h(r,t)}{\partial r}ar + \frac{\partial^2 h(r,t)}{\partial r^2}\,b(r) \tag{3.18}$$

In this section, we present the existence and the uniqueness of the new model using the fundamental theorem of calculus and the fixed-point theorem. Thus, applying the fundamental theorem of calculus, we get:

$$\int_0^t \frac{\partial h}{\partial l} dl = \int_0^t f(h,l)\, dl \tag{3.19}$$

Thus,

$$h(r,t) - h(r,0) = \int_0^t f(h,l)\, dl \tag{3.20}$$

We now define a Banach space given as:

$$I_{a,b} = \overline{I_a[t_0]} \,.\, \overline{I_b(h_0)} \tag{3.21}$$

Where,

$$\overline{I_b(t_0)} = [t_0 - a, t_0 + a] \tag{3.22}$$

$$\overline{I_b[h_0]} = [h_0 - b, h_0 + b] \tag{3.23}$$

$$\Gamma\, I_{a,b} \to I_{a,b} \tag{3.24}$$

$$h \to \Gamma\, h = h(r,0) + \int_0^t f(h,l)\, dl \tag{3.25}$$

$$\|l(t)\|_\infty = \sup_{t \in I_a} |l(t)| \tag{3.26}$$

$$M = Sup\, |f(h,l)| \tag{3.27}$$

Firstly, we want to prove that Γ is well defined that, we need to find the condition for;

$$\|\Gamma h - h_0\|_\infty < b \tag{3.28}$$

$$\| \Gamma\, h - h_0 \|_\infty = \left\| \int_0^t f(h,l)\, dl \right\|_\infty \tag{3.29}$$

$$\leq \int_0^t \|f(h,l)\|_\infty\, dl \tag{3.30}$$

$$\leq \int_0^t M\, dl \tag{3.31}$$

$$\leq M \int_0^t dl \tag{3.32}$$

$$\leq M\, T_{max} \tag{3.33}$$

$\| \Gamma\, h - h_0 \|_\infty \leq M\, T_{max} < b \Rightarrow T_{max} < \frac{b}{M}$ so Γ is well defined if $T_{max} < \frac{b}{M}$.

Secondly, we now prove that Γ has Lipschitz condition, that;

$$let\ h_1; h_2\ \epsilon\ I_{a,b}$$

We then evaluate the following

$$\|\Gamma\, h_1 - \Gamma\, h_2\, \|_\infty$$

Where,

$$\Gamma\, h_1 - \Gamma\, h_2 = h_0 + \int_0^t f(h_1, l)\ dl - h_0 - \int_0^t f(h_2, l) dl \tag{3.34}$$

$$= \int_0^t f(h_1, l)\, dl - \int_0^t f(h_2, l)\, dl \tag{3.35}$$

$$\left\| \int_0^t \big(f(h_1, l) - f(h_2, l)\big) dl \right\|_\infty \tag{3.36}$$

$$f(h_1, l) - f(h_2, l) = a(r) \frac{\partial h_1}{\partial r} + \ b(r) \frac{\partial^2 h}{\partial r^2} - a(r) \frac{\partial h^2}{\partial r} - b(r) \frac{\partial^2 h_2}{\partial r^2} \tag{3.37}$$

$$= a(r) \frac{\partial}{\partial r} (h_1 - h_2) + b(r) \frac{\partial^2}{\partial r^2} (h_1 - h_2) \tag{3.38}$$

$$\left\| \int_0^t \big(f(h_1, l) - f(h_2, l)\big)\, dl \right\|_\infty$$

$$= \left\| \int_0^t [a(r) \frac{\partial}{\partial r} (h_1 - h_2) + \ b(r) \frac{\partial^2}{\partial r^2} (h_1 - h_2)]\, dl \right\|_\infty \tag{3.39}$$

$$\left\| \int_0^t (a(r) \frac{\partial}{\partial r} (h_1 - h_2) + b(r) \frac{\partial^2}{\partial r^2} (h_1 - h_2) \right\|_\infty dl$$

$$\leq \int_0^t \left\| a(r) \frac{\partial}{\partial r} (h_1 - h_2) + b(r) \frac{\partial^2}{\partial r^2} (h_1 - h_2) \right\|_\infty dl \tag{3.40}$$

$$\leq \int_0^t \left\{ |\, a(r)| \, \left\| \frac{\partial}{\partial r}(h_1 - h_2) \right\|_\infty + |b(r)| \, \left\| \frac{\partial^2}{\partial r^2}(h_1 - h_2) \right\|_\infty \right\} dl \tag{3.41}$$

$$\int_0^t [|a(r)| \propto_1 \|h_1 - h_2\|_\infty + |b(r)| \propto_2^2 \|h_1 - h_2\|_\infty] \, dt \tag{3.42}$$

$$\leq (\, |a(r)| \propto_1 + \propto_2^2 |b(r)|) \, T_{max} \, \| \, h_1 - h_2 \, \|_\infty \tag{3.43}$$

$$\| \, \Gamma \, h_1 - h_2 \, \|_\infty \leq K \, \| \, h_1 - h_2 \, \| \tag{3.44}$$

Where,

$$K = T_{max}\left[|\, a(r)| \;\propto_1 + \propto_2^2 \left|| \, b(r)|\right|\right] \tag{3.45}$$

Γ is Lipchitz operator Γ,

Γ will be contraction if:

$$K < 1 \Rightarrow T_{max}\left[|\, a(r)| \;\propto_1 + \propto_2^2 \left|| \, b(r)|\right|\right] < 1 \tag{3.46}$$

This means that,

$$\Rightarrow T_{max} < \frac{1}{T_{max}\left[|\, a(r)| \;\propto_1 + \propto_2^2 \left|| \, b(r)|\right|\right]} \tag{3.47}$$

Γ is a contraction and well-defined if $T_{max} < \min[\frac{1}{|\, a(r) \,|\propto_1 + |\, b(r) \,|\propto_2^2}, \frac{b}{M}]$.

Therefore, if the below inequality holds

$$T_{max} < \min\left[\frac{1}{|\, a(r) \,| \;\propto_1 + |\, b(r) \,| \propto_2^2}, \frac{b}{M} \right] \tag{3.48}$$

The defined operator Γ has a unique exact solution. The above completes the proof.

3.1 DERIVATION OF EXACT SOLUTION

In the following subsection, we are going to derive the exact analytical solution of a groundwater flow equation for a confined aquifer, using the Boltzmann transform.

The derivation of exact analytical solution of the groundwater flow equation for confined aquifer is as follows:

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}\left[1+\frac{\Delta r}{r}\right] \tag{3.49}$$

Initial conditions:

$$h(r,0)=0,$$

Boundary conditions:

$$Lim\frac{\partial h}{\partial r}=-\frac{Q}{2\pi r}$$

$$r\to 0$$

According to the Boltzmann transformation, the reduction of an equation from two dimensions to one dimension:

Let $$\eta=\frac{r^2}{t}$$

We then change everything in terms of η.

$$\frac{\partial h}{\partial t}=\frac{\partial h}{\partial \eta}.\frac{\partial \eta}{\partial t}=\frac{-r^2}{t^2} \tag{3.50}$$

$$\frac{\partial h}{\partial r}=\frac{\partial h}{\partial \eta}.\frac{\partial \eta}{\partial r}=\frac{2r}{t}.\frac{\partial h}{\partial \eta} \tag{3.51}$$

$$\frac{\partial h}{\partial r^2}=\frac{\partial}{\partial \eta}\left(\frac{2r}{t}.\frac{\partial h}{\partial \eta}\right).\frac{\partial \eta}{\partial r} \tag{3.52}$$

$$=\frac{\partial^2 h}{\partial \eta^2}\left(\frac{2r}{t}.\frac{2r}{t}\right) \tag{3.53}$$

$$=\frac{4r^2}{t^2}.\frac{\partial^2 h}{\partial \eta^2} \tag{3.54}$$

By replacing everything back into equation (3.49), we get:

$$\frac{-S}{T}.\frac{r^2}{t^2}.\frac{\partial h}{\partial \eta}=\frac{1}{r}.\frac{2r}{t}.\frac{\partial h}{\partial \eta} + \frac{4r^2}{t^2}.\frac{\partial^2 h}{\partial \eta^2}(r+\frac{\Delta r}{r}) \tag{3.55}$$

$$= \frac{2}{t}.\frac{\partial h}{\partial \eta} + \frac{4r^2}{t^2}.\frac{\partial^2 h}{\partial \eta^2} \tag{3.56}$$

Putting everything together, we get:

$$\left(1 + \frac{\Delta r}{r}\right)\frac{4r^2}{t^2}.\frac{\partial^2 h}{\partial \eta^2} = \frac{-\partial h}{\partial \eta}\left(\frac{S}{T}.\frac{r^2}{t^2} + \frac{2}{t}\right) \tag{3.57}$$

By simplification:

$$\left(1 + \frac{\Delta r}{r}\right)\frac{4r^2}{t}.\frac{\partial^2 h}{\partial \eta^2} = \frac{-\partial h}{\partial \eta}\left(\frac{S}{T}.\frac{r^2}{t} + 2\right) \tag{3.58}$$

Since $\frac{r^2}{t} = \eta$, we get:

$$\left(1 + \frac{\Delta r}{r}\right)4\eta\frac{\partial^2 h}{\partial \eta^2} = \frac{-\partial h}{\partial \eta}\left(\frac{S}{T}\eta + 2\right) \tag{3.59}$$

$$\frac{\Delta r}{r} = \beta$$

Therefore,

$$(1 + \beta)\ 4\eta\frac{\partial^2 h}{\partial \eta^2} = \frac{-\partial h}{\partial \eta}\left(\frac{S}{T}\eta + 2\right) \tag{3.60}$$

We then divide everything by $(1 + \beta)\ 4\eta$:

$$\frac{\partial^2 h}{\partial \eta^2} = \sigma\frac{1}{1 + \beta}.\frac{\partial h}{\partial \eta}\left(\frac{S}{4T} + \frac{1}{2\eta}\right) \tag{3.61}$$

$Let\ v = \frac{\partial h}{\propto \eta}$

$$v' = \sigma\frac{1}{1 + \beta}\left(\frac{S}{4T} + \frac{1}{2\eta}\right)V \tag{3.62}$$

$$\frac{v'}{v} = \sigma\frac{1}{1 + \beta}\left(\frac{S}{4T} + \frac{1}{2\eta}\right) \tag{3.63}$$

By integration, we get:

$$\ln v = \sigma\int_0^{\eta}\frac{1}{1 + \beta}\left(\frac{S}{4T} + \frac{1}{2}k\right)dk \tag{3.64}$$

$$\ln v = \sigma \frac{1}{1+\beta}\left(\frac{S\eta}{4T} + \frac{1}{2}\ln \eta\right) + C \tag{3.65}$$

$$\ln v = \sigma \frac{1}{1+\beta}\left(\frac{S\eta}{4T} + \frac{1}{2}\ln \eta\right) + C \tag{3.66}$$

$$v = \exp(c)\exp\left[\sigma \frac{1}{1+\beta}\left(\frac{S\eta}{4T} + \frac{1}{2} ln\, \eta\right)\right] \tag{3.67}$$

$$\frac{\partial h}{\partial \eta} = Dexp\left[\sigma \frac{1}{1+\beta}\left(\frac{S\eta}{4T} + \frac{1}{2}\ln \eta\right)\right] \tag{3.68}$$

Using the initial conditions, the first derivative $\frac{1}{r}$ turns to zero, which is equal to $-\frac{Q}{2\pi r}$.

$$\eta = \frac{r^2}{t}, r \to 0, \eta \to 0$$

By replacing η by zero, you obtain the following:

$$-\frac{Q}{2\pi T} = D$$

By replacing D from equation (3.68), we get the following:

$$\frac{\partial h}{\partial \eta} = -\frac{Q}{2\pi T}\exp\left[\sigma \frac{1}{1+\beta}\left(\frac{S\eta}{4T} + \frac{1}{2} ln\, \eta\right)\right] \tag{3.69}$$

$$\frac{\partial h}{\partial \eta} = -\frac{Q}{2\pi T}\exp\left[\sigma \frac{1}{1+\beta}.\frac{S\eta}{4T}\right]\exp\left[\sigma \frac{1}{1+\beta}.\frac{1}{2} ln\, \eta\right] \tag{3.70}$$

$Let\ \sigma \frac{1}{1+\beta} = \propto$

$$\frac{\partial h}{\partial \eta} = -\frac{Q}{2\pi T}\exp\left[-\frac{S\eta}{4T \propto}\right]\exp\left[-\frac{1}{2} \propto ln\, \eta\right] \tag{3.71}$$

Rearranging $\exp\left[-\frac{1}{2} ln\, \eta\right]$, we get:

$$= -\frac{Q}{2\pi T}\exp\left[-\frac{S\eta}{4T \propto}\right]\exp\left[ln\left(\eta^{-\frac{1}{2}\propto}\right)\right] \tag{3.72}$$

$$\frac{\partial h}{\partial \eta} = -\frac{Q}{2\pi T}.\frac{1}{\eta^{2\propto}}\exp\left[-\frac{S\eta}{4T \propto}\right]$$

(3.73)

We integrate:

$$h(\eta) = -\int_0^{\eta} \frac{Q}{2\pi T} \cdot \frac{1}{k^{2\propto}} \exp\left[-\frac{Sk}{4T \propto}\right] dk + B \tag{3.74}$$

Using the initial conditions that says:

$$t \to 0, \qquad we\ get\ h\ (r, 0) = 0$$

$$t \to 0,\ \ \eta = \frac{r^2}{t} \to \infty$$

$$0 = -\int_0^{\infty} \frac{Q}{2\pi T} \frac{1}{k^{2\propto}} \exp\left[-\frac{Sk}{4T \propto}\right] dk + B \tag{3.75}$$

$$B = \int_0^{\infty} \frac{Q}{2\pi T} \cdot \frac{1}{k^{2\propto}} \exp\left[-\frac{Sk}{4T \propto}\right] dk \tag{3.76}$$

By replacing equation (3.75) and (3.76) into equation (3.74), we get:

$$h(\eta) = \int_0^{\infty} \frac{Q}{2\pi T k^{2\propto}} \exp\left[-\frac{Sk}{4T \propto}\right] dk - \int_0^{\eta} \frac{Q}{2\pi T k^{2\propto}} \exp\left[-\frac{Sk}{4T \propto}\right] dk \tag{3.77}$$

Therefore,

$$h(\eta) = \frac{Q}{2\pi T} \int_{\eta}^{\infty} \frac{\exp\left[-\frac{Sk}{4T \propto}\right]}{\sqrt[\propto]{k}} dk \tag{3.78}$$

$$Let\ k = \mathfrak{r}^2, \quad dk = 2\mathfrak{r}\, d\mathfrak{r}$$

Thus, we get:

$$= \frac{Q}{2\pi T} \int_{\eta}^{\infty} \frac{\exp\left[\frac{-S\mathfrak{r}^2}{4T \propto}\right]}{\mathfrak{r}^{\propto -1}} . 2 \propto d\mathfrak{r} \tag{3.79}$$

$$= \frac{\frac{Q}{\pi T} \exp\left[-\frac{S\mathfrak{r}^2}{4T \propto}\right]}{\mathfrak{r}^{\propto -1}} d\mathfrak{r} \tag{3.80}$$

$$u = S\mathfrak{r}^2, du = \frac{2S\mathfrak{r} d\mathfrak{r}}{4T \propto} \Longrightarrow d\mathfrak{r} = 2\frac{T}{S}\frac{\propto}{\mathfrak{r}} d(u)$$

$$= \frac{\frac{Q}{\pi T}\int_u^{\infty} \exp[-y]\frac{2T \propto}{S\gamma}dy}{\left[\frac{u\,T \propto y}{S}\right]^{\frac{\propto-1}{2}}} \tag{3.81}$$

$$= \frac{Q}{\pi T}\int_u^{\infty} \frac{\exp[-y]}{\left(\frac{u\,T \propto y}{S}\right)^{\propto-1}} . \frac{2T \propto}{S\left(\frac{4T \propto y}{S}\right)^{\frac{1}{2}}}dy \tag{3.82}$$

$$\frac{Q}{\pi T}\int_u^{\infty} \frac{\exp(-y)}{\left(\frac{4T \propto y}{S}\right)^{\frac{\propto}{2}}} . \frac{2T \propto}{S}dy \tag{3.83}$$

$$h(\eta) = \frac{Q}{2\pi T}\left(\frac{1}{\frac{4T \propto}{S}}\right)^{\frac{\propto-1}{2}} \int_u^{\infty} \frac{\exp[-y]}{y^{\frac{\propto}{2}}}dy \tag{3.84}$$

Above is the exact solution of the groundwater flow equation for a confined aquifer.

CHAPTER FOUR: NEW NUMERICAL SCHEME FOR SINGULAR PARTIAL DIFFERENTIAL EQUATION

4.1 INTRODUCTION

In this section, the Mellin transform is going to be used to remove the singularity in the newly developed exact groundwater flow equation in a confined aquifer. The equation then becomes ordinary, wherein we can then use the Adam Bashforth method to the ordinary differential equation in Mellin space. The inverse of Mellin will then be used to get the exact numerical scheme.

4.2 DERIVATION OF THE NEW NUMERICAL SCHEME TO THE EQUATION

The Mellin transform was first introduced by the Finnish mathematician, R.H. Mellin (1854-1933), who was the first to give a systematic formulation of the transformation and its inverse. Working in the theory of special functions, he developed applications to the solution of hypergeometric differential equations and to the derivation of asymptotic expansions. The Mellin contribution gives a prominent place to the theory of analytic functions. Mellin's transformation has proved useful in the resolution of linear differential equations in $x(d/dx)$ arising in electrical engineering by a procedure analogous to Laplace's (Betrand *et al.,* 2000). More recently, traditional applications have been enlarged and new ones are emerging.

Let $f(t)$ be a function defined on the positive real axis $0 < t < \infty$. The Mellin transformation M is the operation mapping the function f into the function F defined on the complex plane by the relation:

$$M[f;s] \equiv F(s) = \int_0^\infty f(t)t^{s-1}\,dt \tag{4.1}$$

The function $F(s)$ is called the Mellin transform of f. In general, the integral does exist only for complex values of $s = a + jb$ such that $a < a_1 < a_2$, where a_1 and a_2 depend on the function $f(t)$ to transform. This introduces what is called the strip of definition of the Mellin transform that will be denoted by $s(a_1, a_2)$.

The following are useful properties of the Mellin transform (Poularikas and Alexander, 1999):

I. Scaling Property

$$M\{t^a f(t); s\} = \int_0^\infty f(t) t^{(s+a)-1}\, dt$$

$$= a^{-s} \int_0^\infty f(x) x^{s-1}\, dx = a^{-s}\, F(s) \tag{4.2}$$

II. Multiplication by t^a

$$M\{t^a f(t); s\} = \int_0^\infty f(t) t^{(s+a)-1}\, dt = F(s+a) \tag{4.3}$$

III. Raising the Independent Variable to a Real Power

$$M\{f(t^a); s\} = \int_0^\infty f(t^a) t^{s-1}\, dt$$

$$= \int_0^\infty f(x) x^{\frac{s}{a}-\frac{1}{a}} \left(\frac{1}{a} x^{\frac{1}{a}-1}\, dx\right) = a^{-1} F\left(\frac{s}{a}\right), a > 0 \tag{4.4}$$

IV. Inverse of Independent Variable

$$M\{t^{-1} f(t^{-1}); s\} = F(1-s) \tag{4.5}$$

V. Multiplication by $\ln t$

$$M\{\ln t\ f(t); s\} = \frac{d}{ds} F(s) \tag{4.6}$$

VI. Multiplication by Power of $ln\, t$

$$M\{(\ln t)^k\, f(t); s\} = \frac{d^k}{ds^k} F(s) \tag{4.7}$$

VII. Derivative

$$M\left[\frac{d^k}{ds^k} f(t); s\right] = (-1)^k (s-k)_k\, F(s-k) \tag{4.8}$$

$$(s-k)_k \equiv (s-k)(s-k+1)\dots(s-1)$$
$$= \frac{(s-1)!}{(s-k-1)!} = \frac{\Gamma(s)}{\Gamma(s-k)} \tag{4.9}$$

VIII. Derivative Multiplied by Independent Variable

$$M\left[t^k \frac{d^k}{ds^k} f(t); s\right] = (-1)^k (s)_k \, F(s)$$
$$= (-1)^k \frac{\Gamma(s+k)}{\Gamma(s)} F(s), (s)_k \tag{4.10}$$
$$= s(s+1)\dots(s+k-1)$$

IX. Convolution

$$M\{f(t)g(t); s\}$$
$$= \frac{1}{2\pi j} \int_{c-j\infty}^{c+j\infty} F(z)G(s-z)\, dz \tag{4.11}$$

X. Multiplicative Convolution

$$M\{fvg\} = M\left[\int_0^\infty f\left(\frac{t}{u}\right) g(u) \frac{du}{u}; s\right] \tag{4.12}$$
$$= F(s)\, G(s)$$

$$M^{-1}\{F(s)\, G(s)\} = \int_0^\infty f\left(\frac{t}{u}\right) g(u) \frac{du}{u} \tag{4.13}$$

XI. Parseval's Formula's

$$\int_0^\infty f(t)\, g(t) = \frac{1}{2\pi j} \int_{c-\infty}^{c+\infty} M\{f; s\}\, M\{g; 1-s\}\, ds \tag{4.14}$$

$$\int_0^\infty f(t)\, g^*(t) t^{2r+1}\, dt \tag{4.15}$$
$$= \int_{-\infty}^\infty M\{f\}(\beta)\, M^*\{g\}(\beta)\, d\beta$$

Where,

$$M\{f\}(\beta) = \int_0^\infty f(t) t^{2\pi j\beta + r}\, dt \tag{4.16}$$

Application of the new numerical scheme to the equation is as follows:

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}\left[1+\frac{dr}{r}\right]$$

The above is the exact solution of the groundwater flow equation in a confined aquifer.

Introducing a small perturbation term $\Delta r = dr = scaling\ constant$

$$\frac{S}{T}.\frac{\partial h}{\partial t}=\frac{\partial h}{r\partial r}+\frac{\partial^2 h}{\partial r^2}\left[1+\frac{\Delta r}{r}\right]$$

By dividing the above equation with $\frac{S}{T}$, we get:

$$\frac{\partial h}{\partial t}(r,t)=\frac{T}{S}.\frac{\partial h}{r\partial r}+\frac{T}{s}.\frac{\partial^2 h}{\partial r^2}\left[1+\frac{\Delta r}{r}\right]$$

$$\frac{\partial h(r,t)}{\partial t}=\frac{T}{S}\frac{\partial h\,(r,t)}{\partial r}a_1(r)+\frac{\partial h^2}{\partial r^2}a_2(r,t) \tag{4.17}$$

We then apply the Mellin transform on both sides of (4.17) in r-direction.

$$M\left(\frac{\partial h(r,t)}{\partial t},P\right)=\frac{T}{S}M\left(\frac{\partial h(r,t)}{\partial r}a_1(r)+\ a_2(r)\frac{\partial^2 h}{\partial r^2}(r,t),P\right) \tag{4.18}$$

$$M=[h(r,t),P]=H(p,t) \tag{4.19}$$

$$\frac{\partial H(p,t)}{\partial t}=\frac{T}{S}M\left(\frac{\partial h(r,t)}{\partial r}a_1(r)+a_2(r)\frac{\partial^2 h}{\partial r^2}(r,t),P\right) \tag{4.20}$$

$$\frac{\partial H(p,t)}{\partial t}=\frac{T}{S}M\left(\frac{\partial h(r,t)}{\partial r}a_1(r)+\ a_2(r)\frac{\partial^2 h}{\partial r^2}(r,t),P\right)$$

$Put\ V(t)=H(P,t)$,

Therefore,

$$\frac{dV(t)}{dt}=F(V(t),t) \tag{4.21}$$

Applying the fundamental theorem of calculus (Batogna and Atangana, 2017), we get:

$$V(t) - V(0) = \int_0^t F\,(V(t), t))\; dt \tag{4.22}$$

$$t_n = n\Delta t \tag{4.23}$$

$$t_{n+1} = (n+1)\Delta t \tag{4.23}$$

$$V(t_n) - V(0) = \int_0^{t_n} F\,(V(t), t)\; dt \tag{4.24}$$

Within $[t_n, t_{n-1}]$ we approximate using the Lagrange interpolation formula to obtain

$$F\big(t, V(t)\big) = P(t) = \frac{t - t_{n-1}}{t_n - t_{n-1}} F\big(t_n, V(t_n)\big) + \frac{t - t_n}{t_{n-1} - t_n} . F\big(t_{n-1}, V(t_{n-1})\big) \tag{4.25}$$

$$t_n - t_{n-1} = \Delta t$$

$$t_{n-1} - t_n = -\Delta t$$

Thus, the approximate polynomial associated to the new equation is given as:

$$P(t) = \frac{t - t_{n-1}}{\Delta t} F\big(t_n, V(t_n)\big) - \frac{t - t_n}{\Delta t} F\big(t_{n-1}, V(t_{n-1})\big) \tag{4.26}$$

Let us put for simplicity $F_n = F\big(t_n, V(t_n)\big)$

$$V(t_n) - V(0) = \int_0^{t_n} \left(\frac{t - t_{n-1}}{\Delta t} F_n - \frac{t - t_n}{\Delta t} F_{n-1}\right) dt \tag{4.27}$$

$$= \frac{F_n}{\Delta t}\int_0^{t_n} (t - t_{n-1})\; dt - \frac{F_{n-1}}{\Delta t}\int_0^{t_n} (t - t_n)\; dt \tag{4.28}$$

$$V(t_n) - V(0) = \frac{F_n}{\Delta t}\left[\frac{t^2}{2} - t t_{n-1}\right]_0^{t_{n+1}} - \frac{F_{n-1}}{\Delta t}\left[\frac{t^2}{2} - t_n t\right]_0^{t_n} \tag{4.29}$$

$$\frac{F_n}{\Delta t}\left[\frac{t_n^2}{2} - t_n t_n\right] - \frac{F_{n-1}}{\Delta t}\left[\frac{t_n^2}{2} - t_n t_n\right] \tag{4.30}$$

$$\frac{F_n}{\Delta t}\left[-\frac{1}{2}t_n^2\right]-\frac{F_n}{\Delta t}\left[-\frac{1}{2}t_n^2\right] \tag{4.31}$$

$$=\frac{\frac{1}{2}t_n^2}{2\Delta t}[F_{n-1}-F_n] \tag{4.32}$$

$$=\frac{(\Delta t)^2 n^2}{2\Delta t}[F_{n-1}-F_n] \tag{4.33}$$

Therefore,

$$V(t_n)-V(0)=\frac{F_n}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}-(\Delta \mathrm{t})^2\{n(n-1)\}\right]+\frac{F_{n-1}}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}\right] \tag{4.34}$$

Applying the inverse Mellin transform, we get:

$$h(r,t_n)-h(r,0)=M^{-1}\left(\frac{F_n}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}-(\Delta \mathrm{t})^2\{n(n-1)\}\right]+\frac{F_{n-1}}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}\right]\right) \tag{4.35}$$

We now do the approximation in space. We can use Forward Euler or Backward Euler to obtain,

$$x_i-x_{i-1}=\Delta x \tag{4.36}$$

$$h(r_i,t_n)-h(r_i,0)=M^{-1}\left(\frac{F_n{}^i}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}-(\Delta \mathrm{t})^2\{n(n-1)\}\right]+\frac{F_{n-1}^i}{\Delta t}\left[\frac{(n\Delta \mathrm{t})^2}{2}\right]\right) \tag{4.37}$$

$$F(r,t)=\frac{T}{S}\left(\frac{\partial h(r,t)}{\partial r}a_1(r)+\ a_2(r)\frac{\partial^2 h}{\partial r^2}(r,t),P\right) \tag{4.38}$$

Thus letting

$$h(r_i,t_n)=h_i^n \tag{4.39}$$

Replacing equation (4.39), (4.38) into equation (4.37) after re-arranging, we get

$$h_i^n\left[1+\frac{n^2\Delta t}{2\Delta x}\frac{T}{S}a_1(r_i)+\frac{n^2\Delta t}{2(\Delta x)^2}\frac{T}{S}a_2(r_i)\right]$$

$$=h_i^{n-1}\left[\frac{n^2\Delta t}{2\Delta x}\frac{T}{S}a_1(r_i)+\frac{n^2\Delta t}{2(\Delta x)^2}a_2(r_i)\frac{T}{S}\right]$$

$$
\begin{aligned}
&+ h_{i-1}^{n-1}\left[\frac{n^2\Delta t\, T}{2\, S\Delta x}a_1(r_i) + \frac{n^2\Delta t\, T}{(\Delta x)^2}a_2(r_i)\right] \\
&+ h_{i-1}^{n}\left[\frac{n^2\Delta t\, T\, a_1(r_i)}{2\, S\Delta x} + \frac{n^2\Delta t\, T}{(\Delta x)^2}a_2(r_i)\right] \\
&+ h_{i-2}^{n-1}\left[\frac{T}{S(\Delta x)^2}a_2(r_i) - h_{i-2}^{n}\frac{Ta_2(r_i)}{S(\Delta x)^2}\right]
\end{aligned} \tag{4.40}
$$

Above is the exact numerical scheme for singular partial differential equation.

For simplicity, the above equation can be written as:

$$
\begin{aligned}
h_i^n a_1 = h_i^{n-1}a_2 + h_{i-1}^{n-1}a_3 \\
+ h_{i-2}^{n-1}a_4 - h_{i-2}^{n}a_5
\end{aligned} \tag{4.41}
$$

4.3 STABILITY ANALYSIS OF NEW NUMERICAL SCHEME USING VON NEUMANN METHOD

The von Neumann stability method was first developed in Los Alamos during World War 2 by von Neumann and was considered classified until its brief description in Crank and Nicholson (1947) and in a publication by Charney et al (1950). Today it is the most widely used technique for stability analysis throughout the entire world. This method often uses the Fourier analysis and sometimes superposition. It is based on the decomposition of motion into formal nodes. In this method, the growth or decay of perturbations are analyzed from one step to the next and can be put into effect using standard linear algebraic procedures. The method is local in nature. According to Delahaies (2012), the stability of a numerical scheme is associated with propagation of numerical error.

A finite difference scheme is stable if the error stays constant or decrease as the iterative process goes on. On the other hand, if the error grows with time, the scheme tends to be unstable. The von Neumann stability method has limitations: it can be only applied to linear, constant coefficients partial differential equations and neglects boundary conditions. Through linearization, the method can be applied to nonlinear systems.

Composition of the von Neumann stability method involve:

- Substituting the trial function,

$$U_{j,n} = \boldsymbol{\xi^n} e^{iwj} \tag{4.41}$$

  Into the approximate difference scheme and find a characteristic equation for the amplification factor ξ.
- Finding what restrictions on the parameters are required to have $|\boldsymbol{\xi}| \leq 1$: the scheme is von Neumann stable if $|\boldsymbol{\xi}| \leq 1$, and von Neumann unstable if $|\boldsymbol{\xi}| > 1$. When the characteristic equation has multiple roots, it is required to be distinct.

Stability analysis to new numerical scheme is as follows:

$$h_i^n a_1 = h_i^{n-1} a_2 + h_{i-1}^{n-1} a_3 + h_{i-2}^{n-1} a_4 - h_{i-2}^n a_5$$

For stability analysis, we must make sure that

$$for\ all\ n \geq 0$$

$$|h_i^n| < |h_i^0|$$

To do the above, we choose

$$h_i^n = \acute{h}_n \exp[jf_i \Delta r] \tag{4.42}$$

$$h_i^{n-1} = \acute{h}_{n-1} \exp[jf_i \Delta r] \tag{4.43}$$

$$h_{i-1}^{n-1} = \acute{h}_{n-1} \exp[jf_i (r - \Delta r)] \tag{4.44}$$

$$h_{i-2}^{n-1} = \acute{h}_{n-1} \exp[jf_i (r - 2\Delta r)] \tag{4.45}$$

$$h_{i-z} = \acute{h}_n \exp[jf_i (r - 2\Delta r)] \tag{4.46}$$

We then substitute the above equations to equation (4.40);

$$\begin{gathered} \acute{h}_n \exp[jf_i \Delta r]\, a_1 = \acute{h}_{n-1} \exp[jf_i \Delta r]\, a_2 \\ + \acute{h}_{n-1} \exp[jf_i (r - \Delta r)]\, a_3 \\ + \acute{h}_{n-1} \exp[jf_i (r - 2\Delta r)]\, a_4 \\ - \acute{h}_n \exp[jf_i (r - 2\Delta r)]. \\ \acute{h}_n \exp[jf_i \Delta r]\, a_1 = \acute{h}_{n-1} \exp[jf_i \Delta r]\, a_2 \\ + \acute{h}_{n-1} \exp[jf_i r] \,.\, \exp(-jf_i \Delta r)\, a_3 \end{gathered} \tag{4.47}$$

$$+ \acute{h}_{n-1} \exp(jf_i r) \,.\, \exp(-2jf_i \Delta r)\, a_4 \qquad (4.48)$$
$$- \acute{h}_n \exp(jf_i r) \,.\, \exp(-2jf_i \Delta r) a_5.$$

The above equation is simplified by cancelling out $(jf_i r)$

$$\acute{h}_n a_1 = \acute{h}_{n-1} a_2 + \acute{h}_{n-1} \exp(-jf_i \Delta r)\, a_3$$
$$+ \acute{h}_{n-1} \exp[-2jf_i \Delta r]\, a_4 - \acute{h}_n \exp(-2jf_i \Delta r) a_5 \qquad (4.49)$$
$$\acute{h}_n (a_1 + a_5 \exp(-2jf_i \Delta r)) = \acute{h}_{n-1} (a_2 + a_3 \exp(-jf_i \Delta r))$$
$$+ a_4 \exp(-2jf_i \Delta r) \qquad (4.50)$$

Therefore,

$$\left| \frac{\acute{h}_n}{\acute{h}_{n-1}} \right| < 1 \Longrightarrow \left| \frac{a_2 + a_3 \exp[-jf_i \Delta r] + a_4 \exp[-2jf_i \Delta r]}{a_1 + a_5 \exp[-2jf_i \Delta r]} \right| < 1 \qquad (4.51)$$
$$\left| a_2 + a_3 \exp(-jf_i \Delta r) + a_4 \exp(-2jf_i \Delta r) \right|$$
$$< |a_1 + a_5 \exp[-2jf_i \Delta r]| \qquad (4.52)$$
$$|a_2| + |a_3| + |a_4| < |a_1| + |a_5| \qquad (4.53)$$

By substituting $(a_1, a_2, a_3, a_4, a_5)$ we get

$$\left| \frac{n^2 \Delta t T}{2 \Delta x S} c_1(r_i) \right| + \left| \frac{n^2 \Delta t}{2(\Delta x)^2} c_2(r_i) \frac{T}{S} \right|$$
$$+ \left| \frac{n^2 \Delta t T}{2 S \Delta x} c_1(r_i) + \frac{n^2 \Delta t T}{(\Delta x)^2} c_2(r_i) + \frac{T}{S(\Delta x)^2} c_2(r_i) \right|$$
$$< \left| \frac{1 + n^2 \Delta t}{2 \Delta x} \frac{T}{S} c_1(r_i) + \frac{n^2 \Delta t}{2(\Delta x)^2} \frac{T}{S} c_2(r_i) \right| + \left| \frac{T c_2(r_i)}{S(\Delta x)^2} \right| ! \qquad (4.54)$$

Therefore,

$$\left| \left\{ \frac{n^2 \Delta t T}{2(\Delta x S} c_1(r_i) \right\} \right| + \left| \frac{n^2 \Delta t}{2(\Delta x)^2} c_2(r_i) \frac{T}{S} \right| + \left| \frac{n^2 \Delta t T}{2 S \Delta x} c_1(r_i) \right| + \left| \frac{n^2 \Delta t T}{(\Delta x)^2 S} \right|$$
$$+ \left| \frac{T}{S(\Delta x)^2} c_2(r_i) \right|$$
$$< \left| \frac{1 + n^2 \Delta t}{2 \Delta x} \frac{T}{S} c_1(r_i) \right| + \left| \frac{n^2 \Delta t}{2(\Delta x)^2} \frac{T}{S} (c_2 r_i) \right| + \left| \frac{T c_2}{S(\Delta x)^2} \right| ! \qquad (4.55)$$

$$\frac{n^2\Delta t\ T}{\Delta x\ S}c_1(r_i) + \frac{n^2\Delta t\ T}{S\ (\Delta x)^2}c_2(r_i) < \frac{1 + n^2\Delta t\ T}{2(\Delta x)S}c_1 r_i \tag{4.56}$$

The above equation can be simplified by taking out the common factor,

$$n^2\Delta t\ T\ c_1(r_i) + \frac{n^2\Delta t\ T}{\Delta x}c_2(r_i) < \frac{1 + n^2\Delta t\ T}{2}c_1(r_i) \tag{4.57}$$

We then multiply everything by 2,

$$2n^2\Delta t\ T\ c_i(r_i) - n^2\Delta t\ T\ c_1(r_i) + \frac{2n^2\Delta t\ T}{\Delta x}c_2(r_i) < 1 \tag{4.58}$$

$$n^2\Delta t\ T\ C_1(r_i) + \frac{2n^2\Delta t\ T}{\Delta x}c_2(r_i) < 1 \tag{4.59}$$

We then factorize $N^2\Delta t\ T$,

$$n^2\Delta t\ T[c_1(r_i) + \frac{2c_2(r_i)}{\Delta x}] < 1 \tag{4.60}$$

Then for condition of stability:

$$c_1(r_i) + \frac{2c_2(r_i)}{\Delta x} < \frac{1}{n^{\,2}\Delta t\ T} \tag{4.61}$$

Therefore,

$$\left[\frac{1}{r}\right] + \frac{2\left[1 + \frac{\Delta r}{r}\right]}{\Delta x} < \frac{1}{n\Delta t\ T} \tag{4.62}$$

The above completes the stability.

CHAPTER FIVE: APPLICATION AND DATA

5.1 APPLICATION OF DATA IN GROUNDWATER MODELLING

In groundwater studies, the initial stage of every groundwater investigation and analysis consists of collecting data. Data collection may include collecting existing geological and hydrological data of the site under study. This information includes geology of the area, precipitation, evapotranspiration, abstraction rates, water level, land use, aquifer hydraulics, initial boundary conditions and many more. At times, such data does not exist and this calls for a need to conduct fieldwork. Fieldwork involves going to the actual site and taking measurements such as water levels, temperature, PH and total dissolved solvents. It also incorporates carrying out slug tests, constant rate test and pump test which help understand aquifer hydraulic properties. Measurements, tests and observations are recorded in a field book and this what is termed groundwater data. Groundwater data is collected using pumps, water loggers, temperature meters, PH, EC, and TDS meters. From this data, Other aquifer properties such as storativity, hydraulic conductivity and transmissivity are then obtained by indirect calculations and numerical simulations.

The key question to ask, is the data collected a real representation of reality? In most cases It is not and little is being done to verify such inaccuracy. The following are examples that prove that most data collected in the field are not actual representation of reality.

5.1.1 The Concept of Averaging

Let's take a monitoring exercise that is being conducted for site x. The site has an abstraction borehole and three other observation boreholes within the vicinity of the site as depicted in figure 1. All three observation boreholes will always have a different transmissivity to one another. The question then arises as to which transmissivity will be used to model the system. Do we use the highest or lowest transmissivity values in the system?

If so, is it a real representation of the whole system? Some authors and consultants in the industry have resorted to using the arithmetic mean average of the system which leads us to our second example.

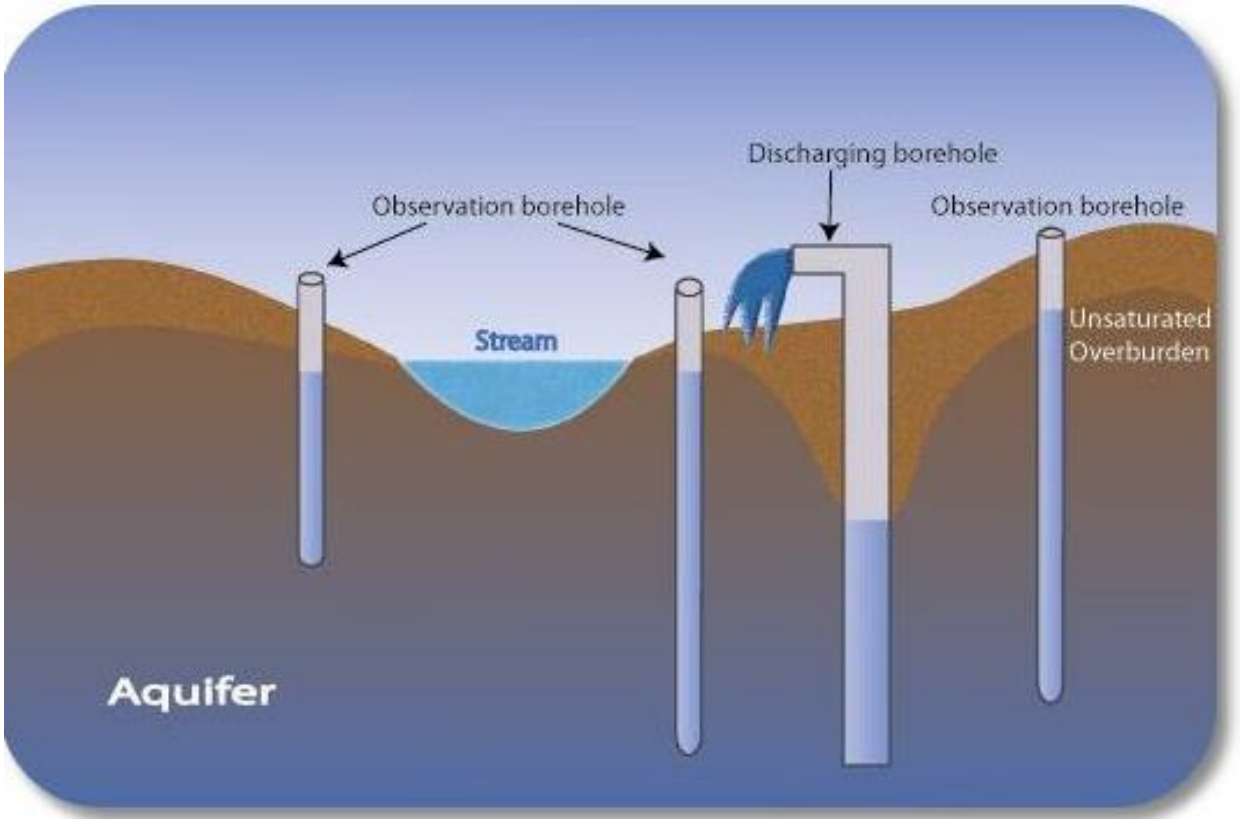

Figure 3: Monitoring System of Site X (Google/Images, 2017).

Let's take a group of five lecturers at a certain department within a university. The first lecturer submitted 15 articles to an international accredited journal for review in a year. The second lecturer submitted 5 articles within the very same year. The third lecturer then submitted only three articles that year. The fourth lecturer submitted two articles while the fifth one did not submit any article that particular year. If we are going to use the arithmetic mean average of articles submitted by the department within that year, we find that at least five articles were submitted per person. Does that give a real representation of reality? It does not and such an example can also be applied in groundwater. Using the arithmetic mean average to represent the groundwater system is not or does not give you the actual representation of reality.

Based on the above examples, we realize that field data cannot always be trusted as it does not depict the actual truth of what is happening in reality. Before using field data, it is important to take as many measurements and try to get a trend. This will further be explained in the following sections.

5.2. APPLICATION OF MATHEMATICS IN DATA PROCESSING

(Nigmatullin et al.,2014) stated that all data can be divided on two large classes: reproducible and unrepeatable data, accordingly. A reproducible data is when a measurement is reproducible if the investigation is repeated by another person, or by using different equipment or techniques, and the same results are obtained. For certain types of data (such as groundwater data) the repetition of the same initial conditions is impossible and therefore requires that special methods for analysis of different time series be used. In some instances, the control variable x is random and the response created by the action of this variable on the area or object studied is also random and so all responses in this instance cannot be reproducible. (Nigmatullin et al.,2014) further suggested the development of a general theory or intermediate model that considers all reproducible data. The theory has to satisfy the following requirements:

- It should give a possibility to express quantitatively a set of the measured functions by means of the unified and common set of the fitting parameters.
- This set of the fitting parameters should form the unified model and many data can be compared in terms of one quantitative “language”. It means that there is a possibility to create general metrological standard for consideration of reproducible data from the unified point of view.
- All calculations that are contained in this general theory should be error controllable.
- It should give a possibility to eliminate the apparatus (instrumental) function and reduce reproducible measurement to an ideal experiment.

The suggested theory can further be expressed in terms of mathematical formulas in the following ways:

If $Pr(x)$ is chosen as the response (measured) function then from the mathematical point of view it implies that the following relationship is satisfied:

$$y_m(x) \cong \Pr(x + m.T_x)$$
$$= \Pr(x + (m-1).T_x, \qquad m = 1,2,\dots.,M. \tag{5.1}$$

Here x is the external (control) variable, T_x is a "period" of experiment expressed in terms of the control variable x.

In equation (5.1), an assumption was made that the properties of the object studied during the period of time T_x is not changed. If $x = t$ corresponds with temporal variable then $T_x = T$ corresponds with the conventional definition of a period. The solution of this functional equation is well-known and (in case of discrete distribution of the given data points $x = x_j, (j = 1, 2, \dots, N)$ coincides with the segment of the Fourier series:

$$\Pr(x) = A_o + \sum_{K=1}^{\infty} \left[Ac_k \cos\left(2\pi K \frac{x}{T_x}\right) + As_K \sin\left(2\pi K \frac{x}{T_x}\right) \right] \tag{5.2}$$

Equation (5.2) shows a segment of the Fourier series since in reality all data points are always discreet and the number of modes which corresponds with the coefficients of the Fourier decomposition is limited. The letter K defines the finite mode. The final mode (K) is chosen from the requirement that it is sufficient to fit experimental data with the given (acceptable) accuracy. The value of K can be calculated (shown in equation 5.8) for the relative error located in the given interval. The acceptable error interval is between 1 percent to ten percent $(1\% - 10\%)$. This interval provides the desired fit of the measured function $y(x)$ to $\Pr(x)$ with initially chosen number of models K figuring from equation (5.2). it is from this relationships that a conclusion can be made. (Nigmatullin *et al.,* 2014) concluded that for an ideally reproducible experiment or data, which satisfies the following conditions: 1. The Fourier transform 2. Can be used as intermediate model (IM) and the number of decomposition coefficients (A_o, Ac_K, As_K) equaled $2K + 1$ can be used as a set of the fitting parameters belonging to the Intermediate Model. The meaning of these coefficients is well-known and actually this set defines approximately the well-known amplitude-frequency response (AFR) associated with the recorded signal $y(x) \approx \Pr(x)$ coinciding with the measured function.

Here we increase only the limits of interpretation of the conventional F-transform with respect to any variable x (including frequency also, if the control variable x coincides with some current) and show that the segment of this transformation can be used for description of an ideal experiment.

Considering a more general equation:

$$F(x + T_x) = aF(x) + b \tag{5.3}$$

The above equation was first developed and used by (Nigmatullin, 2008). The solution of the above equation can be written as follows (Nigmatullin, 2008):

$$a \neq 1 : F(x) \exp\left(\frac{\lambda x}{T}\right) \Pr(x) + C_o$$

$$\lambda = \ln(a)$$

$$C_o = \frac{b}{(1-a)}$$

$$a = 1 : F(x) = \Pr(x) + \frac{bx}{T_x} \tag{5.4}$$

From equation (5.3) the obvious conclusion follows:

$$F(x + mT_x) = aF(x + (m-1)T_x) + b, \qquad m = 1, 2, \dots, M \tag{5.5}$$

It is interpreted as repetition of a set of successive measurements corresponding to an ideal experiment with memory. An assumption was also used about stable properties of the object studied during the period T_x used for the measurements is maintained (constants a and b in equation 5.5 do not depend on time). In reality, this situation cannot be performed because of a set of uncontrollable factors. It is expected that in reality all these constant parameters including the period T_x will depend on the current number of a measurement m

$$y_{m+1}(x) = a_m y_m + b_m \text{ or}$$

$$F\big(x + (m+1)T_x(m)\big) = a_m F\big(x + m.T_x(x)\big)$$

$$+ b_m, m = 1, 2, \dots, M - 1 \tag{5.6}$$

In spite, the solution (5.4) is also valid in this case and in the result of the fitting of the function (5.4) one can express approximately the current measurement $ym(x)$ in terms of the function (5.4) that represents itself the chosen IM. From this IM one can obtain a fitting function for description of reproducible measurements with the shortest memory (5.6). So, for each measurement from expression (5.4) one can derive easily the following fitting function:

$$y_m(x) \cong F_m(x) = B_m + E_m \exp\left(\frac{\lambda_m x}{T_x(m)}\right) + \sum_{K=1}^{N} [Ac_K(m) yc_K(x,m) + As_K(m) ys_K(x,m)]$$

$$yc_K(x,m) = \exp\left(\frac{\lambda_m x}{T_x(m)}\right) cos\frac{(2\pi K x)}{T_x(m)} \qquad (5.7)$$

There is a period of time T that determines the temporal interval when one cycle of measurement is finished. In such a case, the connection between the period T_x defined above and real period T is not known. However, the desired fitting parameter T_x that is shown in equation (5.7) can be calculated from the fitting procedure. In order to find the optimal value of this parameter T_{opt} that provides the accurate fit, it can be seen that this value must be located approximately in the interval $\left[\frac{T_{max}}{2,2T_{maz}}\right]$, where the value of $T_{max}(x)$, in turn, should be defined as $T_{max}(x) = \Delta x.L(x)$. The value Δx is a step of discretization and $L(x) = X_{max} - X_{min}$ is a length of the interval associated with the current discrete variable x. Such observation aid in finding the optimal values of T_{opt} and K from the procedure of minimization of the relative error that always exists between the measured function $y\ (x)$ and the fitting function (5.7):

$$\min[RelErr] = \min\left[\frac{stdev\{y(x) - F(x; T_{opt}, K)\}}{mean|y|}\right].100\%$$

$$1\% < \min[RelErr(K)] < 10\%$$

$$T_{opt} \in \left[\frac{T_{max}}{2, 2T_{max}}\right]$$

$$T_{max} = \left(x_j - x_{j-1}\right).\ L(x) \tag{5.8}$$

Direct calculations show that instead of minimizing the surface $RelErr\ (T, K)$ with respect to the unknown variables T and K one can minimize the cross-section at the fixed value of K. The value of K must satisfy the condition that is given by $1\% < \min[RelErr(K)] < 10\%$.

This procedure should be realized for each successive measurement and therefore the index $m(m = 1, 2, \dots, M)$ is neglected in equation (5.8) in order not to overload this expression with additional parameters. Every person wants to realize the conditions that are close to an ideal experiment with memory expressed by equation (5.3). to achieve this, the set of constants a_m and b_m can be averaged together with the measured functions y_m in order to substitute equation (5.6) by an appropriate equation that is close to the ideal case shown in equation (5.3):

$$Y(x + \langle T_x \rangle) \cong \langle a \rangle Y(x) + \langle b \rangle$$

$$Y(x + \langle T_x \rangle) = \frac{1}{M-2} \sum_{m=2}^{M} y_m(x)$$

$$Y(x) = \frac{1}{M-2} \sum_{m=1}^{M-1} y_m\,(x) \tag{5.9}$$

The averaged functions that are obtained from the given set of the reproducible measurements are defined by the second row of equation (5.9). (Nigmatullin *et al.*, 2014) defined this functional equation as the reduced experiment to its mean values (REMV). It can be seen that constants a_m and b_m are calculated from equation (5.6) as neighboring slopes and intercepts:

$$a_m = slope(y_{m+1}, y_m)$$

$$b_m = intercept\left(y_{m+1}, y_m\right)$$

$$M = 1, 2, \dots, M-1$$

$$\langle a \rangle = \frac{1}{M-1} \sum_{m=1}^{M-1} a_m$$

$$\langle b \rangle = \frac{1}{M-1} \sum_{m=1}^{M-1} b_m \tag{5.10}$$

The set of numbers entering in equation (5.9) should be equal $M-1$. (Nigmatullin *et al.,* 2014) elaborated that all the total set of measurements are necessary to justify the functional equation (5.6).

The shortest memory cannot be realized for every experiment. Instead of equation (5.6) showing the realization of the simplest case between the neighboring measurements it is necessary to consider an ideal situation when the memory covers L neighboring measurements (Nigmatullin *et al.,* 2014). In such instances, we get:

$$F(x + LT_x) = \sum_{l=0}^{L-1} a_l \, F(x + T_x) + b \tag{5.11}$$

The set of parameters a_l and b are easily calculated by the Linear Least Square Method (LLSM) if we assume that $L = M$, where M corresponds with the last measurement. The true value of L cannot be calculated and as such, there is a gap in knowledge. The measurement process that takes place during the interval $[(L-1)T_x, LT_x]$ partially depends on the measurements that have been taken on the previous temporal intervals $[LT_x, (l+1)T_x]$ with $L = 0, 1, \dots, L-2$. The set of constants $[a_l](l = 0, 1, \dots, L-1)$ can be quantitatively interpreted as the influence of a memory between the successive measurements. The solution of equation (5.11) can be written in two forms and was first regarded in 2008 (Nigmatullin, 2008):

$$(A) \sum_{l=0}^{L-1} a_l \neq 1 : F(x) = \sum_{l=1}^{L} (K_l)^{\frac{x}{T_x}} Pr_l\,(x) + c_0$$

$$c_0 = \frac{b}{L-1}, 1 - \sum_{l=0}^{L-1} a_l$$

$$(B) \sum_{l=0}^{L-1} a_l = 1 : F(x) = \sum_{l=1}^{L} (K_l)^{\frac{x}{T_x}} Pr_l(x) + c_1 \frac{x}{T_x}$$

$$c_1 = \frac{b}{l-1}.\ L - \sum_{l=0}^{L-1} l.\, a_l \tag{5.12}$$

The functions $Pr_l(x)$ define a set of periodic functions $(l = 1, 2, \dots, L)$ from equation (5.2), the values K_l corresponds with the roots of the characteristics polynomial:

$$P(K) = K^L - \sum_{l=0}^{L-1} a_l K^l = 0 \tag{5.13}$$

(Nigmatullin *et al.,* 2014) stressed that these roots can either be positive, negative, *g*-fold degenerated (with the value of the degeneracy *g*) and complex conjugated. It should be noted that B in equation (5.12), one of the roots K_l corresponds with the unit value $(K_1 = 1)$ that leads to the pore periodic solution. The finite set of the unknown periodic functions $Pr_l\ (x, T_x)(l = 1, 2, \dots, L$ is determined by their decomposition coefficients $Ac_K^{(l)}, As_K, L = 1, 2, \dots, L; K = 1, 2, \dots, K$.

$$\begin{aligned} Pr_l\ (x, T_x) = A_0^{(l)} + \sum_{K=1}^{K \gg 1} [Ac_K^{(l)} \cos\left(2\pi K \frac{x}{T_x}\right) \\ + As_K^{(l)} \sin(2\pi K \frac{x}{T_x})] \end{aligned} \tag{5.14}$$

Solution (5.12) has general character and other roots from algebraic equation (5.13) can modify the convectional solution. All reproducible measurements having a memory associated with L neighboring measurements should satisfy to the following functional equation:

$$\begin{aligned} y_m(x) &\cong F(x + (L+m)T_x(m)) \\ &= \sum_{l=0}^{L-1} a_l^m\, F\big(x + (L+m)T_x(m)\big) \\ &\quad + b, \qquad m = 1, 2, \dots, M. \end{aligned} \tag{5.15}$$

A possible averaging procedure that can be applied for calculation of the mean functions is shown in equation (5.16). The functional equations (5.16) and (5.11) are similar to each other but do not necessarily mean the same. Equation (5.11) is associated with the ideal experiment with memory while equation (5.16) describes the typical situation of the real experiment when random behavior of the initial measured functions is reduced to tis successive mean values (Nigmatullin, 2014).

In reality, it is always desirable to get the minimal value of L, as L increases the number of the fitting parameters that are required during the final fitting of the measured function. Equation (16) can be clearly understood and corresponds to the linear presentation of a possible memory that may exist between repeated measurements after averaging procedure. (Nigmatullin *et al.,* 2014) demonstrated how to eliminate the apparatus function and reduce the set of the real reproducible measurement to an ideal experiment containing the set of periodic functions only. In equation (5.11) it can be observed that the functions$F(x), F(x+T), \dots, F(x+(L-1)T)$ are linear independent and available from experimental measurements. We get the following linear equations:

$$F(x) = \sum_{l=1}^{L} EP_l\,(x) + c_0$$

$$F(x+T) = \sum_{l=1}^{L} K_l\, EP_l(x) + c_0$$

$$F(x+(L-1)T = \sum_{l=1}^{L} K_l^{L-1}\, EP_l\,(x) + c_0$$

$$EP_l(x) = (K_l)^{\frac{x}{T_x}} Pr_l\,(x), \qquad l = 0, 1, \dots, L-1 \tag{5.16}$$

It is through these linear equations that an unknown function $EP_l(x)$ may be found and then restore the unknown periodic functions $Pr_l(x)$. It then becomes possible to reduce a number of reproducible measurements which were early shown in the frame of the desired intermediate model and corresponds to the Prony's decomposition to an ideal experiment. The L-th order of equation (5.17) does not equal to zero if all roots of equation (5.13) are not the same. This gives the ideal periodic function that corresponds to reduction of the real set of measurements to an ideal experiment:

$$Pf(x) = \sum_{l=0}^{L-1} Pr_l\,(x) \tag{5.17}$$

The above equation is very important and can serve as the link between theory and practical. From equation (5.4) we get:

$$\langle a\rangle \neq 1, \mathrm{Pr}(x) = (\langle a\rangle)^{-\frac{x}{T_x}}\left[y(x) - \frac{\langle b\rangle}{1-\langle a\rangle}\right]$$

$$\langle a\rangle = 1, \mathrm{Pr}(x) = Y(x) - \langle b\rangle\left(\frac{x}{T_x}\right) \tag{5.18}$$

The above formulas eliminate the equipment function based on the demonstrated assumptions in equation (5.9) and equation (5.16). The solution for case B is important and similar to linear equation (5.17) with replacement of the left-hand side by the functions:

$$\Phi(\mathrm{x} + \mathrm{lT}) = \mathrm{F}(\mathrm{x} + \mathrm{lT}) - c_1\left(\frac{x}{T} + l\right)$$

$$l = 0{,}1, \ldots, L-1 \tag{5.19}$$

According to (Nigmatullin *et al.,* 2014) attentive analysis of many data prompts the efficiency of the following simplified algorithm:

- From available set of data, one can calculate the mean measurement:

$$\langle y(x)\rangle = \frac{1}{M}\sum_{m=1}^{M} y_m\,(x) \tag{5.20}$$

  And the distributions of the corresponding slopes and intercepts that demonstrates marginal measurements having a maximal deviation from its mean value:

$$SL_m = slope\ (y_m(x), \langle y(x) \rangle),$$
$$Int_m = intercept\ (y_m(x), \langle y(x) \rangle \tag{5.21}$$

- From these distributions one can find the measured functions having maximal deviations and form two limits (maximal deviations from both sides with respect to mean function).

$$\langle y(x) \rangle = a_1\, yup(x) + a_0\, ydn(x) + b \tag{5.22}$$

- The case of the reduced memory and marginal functions $yup(x)$, $ydn(x)$ describe the limits of the statistical cluster on two opposite limits. The coefficients $\{a_0, 1, b\}$ are found from equation (5.22) by the Linear Least Square Method (LLSM).
- The desired roots $K_{1,2}$ are found from the quadratic equation:

$$K^2 - a, K - a_0 = 0 \tag{5.23}$$

The fit of the function $ydn(x)$ to the Prony's decomposition allows finding the optimal value of T_x.

From the above demonstrations and explanations, we realize that going to the field and collected data is not sufficient enough. If not processed, such data can be very misleading and far from reality. It is important to make sure that the data collected follows a similar trend, fits to the best fit model and the percentage error calculated is between $1\% - 10\%$. If this procedure is not followed then data collection tends to be a fruitless exercise.

5.3 INTERPOLATION OF DATA

In numerical analysis, interpolation is a method of constructing new data points within the range of a distinct set of known data points. During data collection, one often has many data points, obtained through sampling, which represent the values of a function for a limited number of values of the independent variable. Such data points are required and often used to interpolate the value of that function for an intermediate value of the interdependent variable (Wikipedia, 2016). There are different kinds of interpolation methods, as stated below. When choosing an interpolation method to use, one needs to determine how accurate is the method? Is it not expensive? Number of data points needed? Smoothness of the interpolant.

5.3.1 Linear Interpolation

Linear interpolation is the simplest interpolation method. Applying linear interpolation to a sequence of points results in a polygonal line where each straight-line segment connects two consecutive points of the sequence. Therefore, every segment (P, Q) is interpolated independently as follows (Katti *et al.,* 2008; Rahul *et al.,* 2008):

$$P(t) = (1 - t).P + t.Q \tag{5.24}$$

Where $t \in [0,1]$. By varying t from 0 to 1 we get all the intermediate points between P and Q. Note that $P(t) = P$ for $t = 0$ and $P(t) = Q$ for $t = 1$. For values of $t < 0$ and $t > 1$ result in extrapolation, that is, we get points on the line defined by P, Q but outside the segment (P, Q).

Linear interpolation can be defined in more mathematical terms.

Definition 1: A linear interpolation $f: [0,1] \rightarrow \mathbb{R}^n$, $t \mapsto f(t) = (f, (t), \dots, f_n(t)$ is an affine transformation from a unit interval $[0,1]$ to a straight-line segment in $\mathbb{R}^n$, where $f_1(t)$,…,$f_n(t)$ are the function components of f along each coordinate axis (Katti *et al.,* 2008; Rahul *et al.,* 2008).

By definition, an affine transformation preserves barycentric combinations. Therefore, if $t \in [0,1]$ is defined as a barycentric combination of the points $0,1 \in \mathbb{R}$

$$t = \alpha_0.0 + \alpha_1.1, \text{ with } \alpha_0 + \alpha_1 = 1$$

Then

$$f(t) = \alpha_0.f(0) + \alpha_1.f(1), \text{ with } f(0), f(1) \in \mathbb{R}^n$$

$$\text{With } \alpha_0 = 1 - t \text{ and } \alpha_1 = t.$$

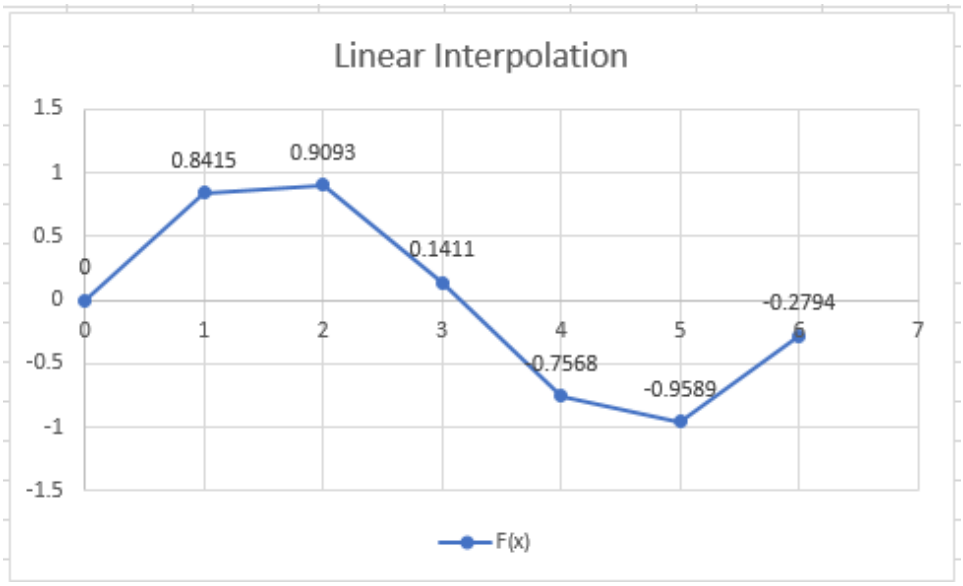

Figure 4: Plot of data with Linear Interpolation imposed.

5.3.2 Piecewise Constant Interpolation

One of the simplest technique of interpolation is to locate the nearest data value, and assign the same value as the previous one as shown in figure 2. In simple problems, this method is mostly not used, as linear interpolation method is as easy but in cases of complex variable interpolation, piecewise constant interpolation is the favored method due to its efficiency and its simplicity.

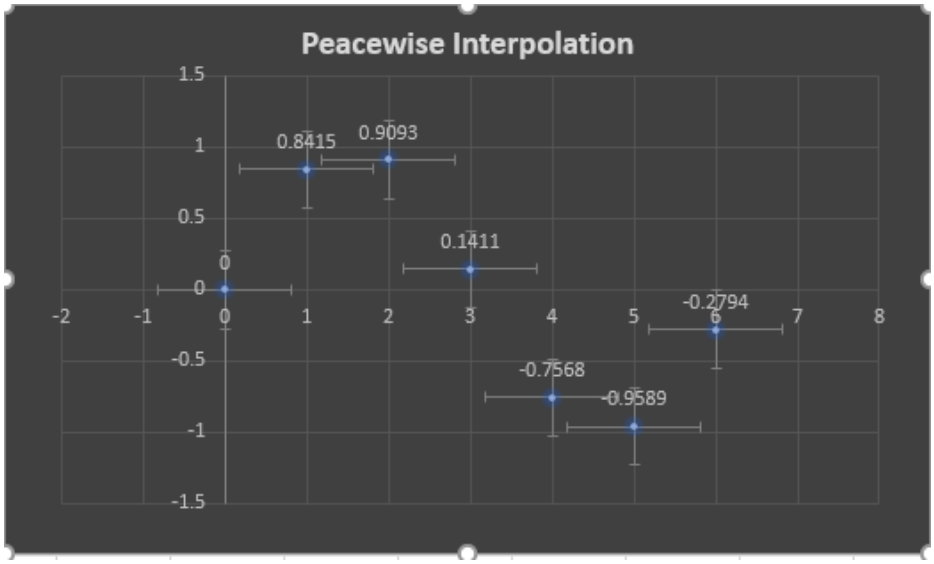

Figure 5: Plot of the data with Piecewise Constant Interpolation applied.

5.3.3 Polynomial Interpolation

Polynomial interpolation is a generalization of linear interpolation. Since linear interpolation is a linear function, it is replaced with a polynomial of higher degree. If we have n data points, there is exactly one polynomial of degree at most $n - 1$ going through all the data points as shown in figure 3. The interpolation error is proportional to the distance between the data points to the power n.

Furthermore, the interpolant is a polynomial and thus infinitely (Wikipedia, 2016). It is in this regard that polynomial interpolation is advantageous over linear interpolation.

Disadvantages of polynomial interpolation include:

- It is computationally expensive to calculate interpolating polynomials.
- Often exhibits oscillatory artifacts at the end points.

Polynomial interpolation can estimate local maxima and minima that are outside the range of the samples, unlike linear interpolation. However, these maxima and minima may exceed the theoretical range of the function i.e. a function that is always positive may have interpolant with negative values (Wikipedia, 2016). Spline interpolation overcomes such setbacks.

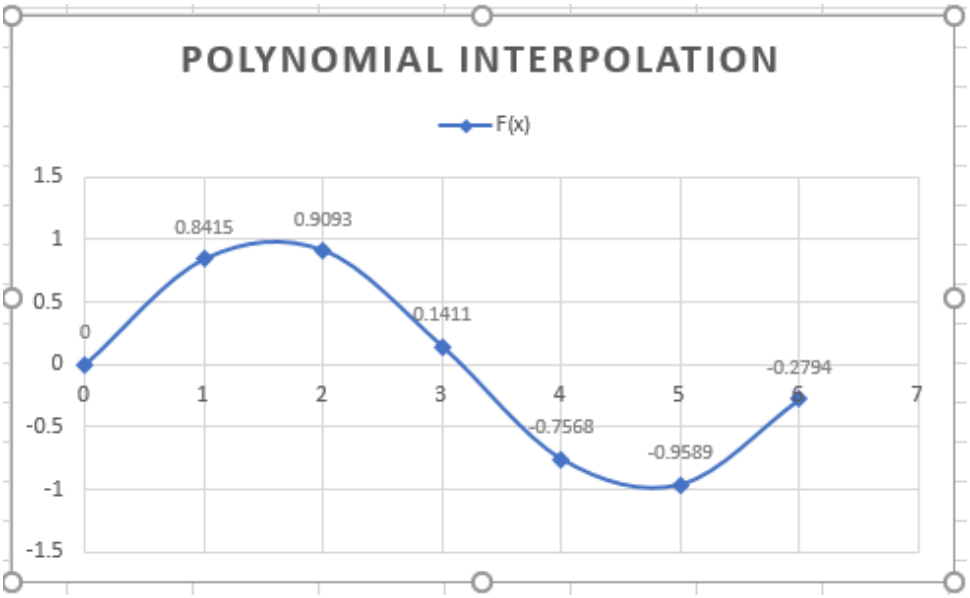

Figure 6: Plot of the data with Polynomial Interpolation applied.

5.3.4 Spline Interpolation

Note that linear interpolation uses a linear function for each of intervals X_k, X_{k+1}. Whereas, spline interpolation uses low-degree polynomials in each of the intervals, and chooses the polynomial pieces such that they fit smoothly together. The resulting function is called a spline. For example, the natural cubic spine is piecewise cubic and twice continuously differentiable. Moreover, its second derivative is zero at the end points (Wikipedia, 2016). Spline interpolation incurs a smaller error than linear interpolation and the interpolant is smoother. In spline interpolation, it is much easier to evaluate the interpolant than the high degree polynomials used in polynomial interpolation.

5.3.5 Interpolation Via Gaussian Processes

This is a powerful non-linear interpolation tool. It is equivalent to many popular interpolation tools. Gaussian processes can be used for fitting an interpolant that passes exactly through the given data and also for regression (fitting a curve through noisy data). Gaussian process regression is also known as Kriging.

5.3.6 Other Forms of Interpolation

Other forms of interpolation can be constructed by picking a different class of interpolants. Examples of other forms of interpolation include:

- Interpolation by rational functions using Pade approximant.
- Interpolation by trigonometric polynomials using Fourier series.
- The Whittaker-Shannon interpolation formula can be used if the number of data points is infinite.

However, multivariate interpolation is the interpolation of functions of more than one variable. Such technique includes Bilinear interpolation and Bicubic interpolation in two dimensions, and trilinear interpolation in three dimensions. This type of interpolation may be applied to gridded or scattered data.

5.4 APPLICATION OF INTERPOLATION IN GROUNDWATER

Interpolation in groundwater is used for analyzing groundwater flow and analyzing groundwater flow and physiochemical parameter distribution. There are areas in which observations and measurements cannot be made and leads to geostatistical methods being employed to determine the values of such areas where measurements were not made. In some instances, people choose to measure groundwater levels and parameters at random locations in the field with the hope of interpolating whatever values and everything happening within the sampled or measured data points. Therefore, the accuracy of such interpolation will determine how accurate is the model output. The following is an example of an interpolation techniques and how it is used in groundwater.

1. Kriging

According to David (1977) kriging is a technique of making optimal, unbiased estimates of regionalized variables at unsampled locations using the structural properties of the semi-variogram and the initial set of data values. This type of interpolation technique considers the spatial structure of the parameter. It is mostly preferred over other interpolation techniques such as arithmetic mean, polynomial interpolation, nearest neighbor method and distance weighted method. It also provides an estimation variance of every estimated point, increasing the accuracy of the interpolant.

Methodology

the initial step of this methodology is calculating the experimental variogram using the following equation which was developed by Kumar and Remadevi (2006):

$$\gamma^*(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [2(x_i) - 2(x_i + h)]^2 \qquad (5.25)$$

Where $\gamma^*(h) =$ estimated value of the semi-variance for lag h; $N(h)$ is the number of experimental pairs separated by vector h; $2(x_i)$ and $2(x_i + h) =$ values of variable 2 at x_i and $x_i + h$, respectively; x_i and $x_i + h =$ position in two dimensions.

The semi-variograms are fitted with various theoretical models like spherical, exponential, gaussian, linear and power by the weighted least square method. The theoretical model that gives the minimum standard error is taken for further analysis. Kriging is then performed at all the data points, ignoring, in turn, one by one. (de Marsily and Ahmed, 1987) explained that differences between estimated and observed values should be summarized using the cross-validation statistics: Mean Error (ME), Mean Squared Error (MSE), Kriged Reduced Mean Error (MRME), and Kringed Reduced Mean Square Error (MRMSE). If the semi-variogram model and kriging procedure sufficiently reproduce the observed value, the error should satisfy the following criteria (Kumar and Remadevi, 2006):

$$ME = \frac{1}{N}\sum_{i=1}^{N}(Z^*(x_i) - Z(x_i)) \cong 0 \tag{5.26}$$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(Z^*(x_i) - Z(x_i))^2 \ minimum \tag{5.27}$$

$$KRME = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{\left(2^*(x_i) - Z(x_i)\right)}{\sigma_{Ki}}\right] \cong 0 \tag{5.28}$$

$$KRMSE = \frac{1}{N}\sum_{i=1}^{N}[\frac{(2^*(x_i) - Z(x_i))^2}{\sigma_{Ki}^2}] \cong 1 \tag{5.29}$$

Where, $Z^*(x_i), Z(x_i)$ and σ_{Ki}^2 are the estimated value, observed value and estimation variance respectively, at points x_i. N is the sample size.

For all interpolation techniques, interpolated value of 2 at any point X_0 is given as the weighted sum of the measured value:

$$Z^* = (X_0) = \sum_{i=1}^{N}\lambda_i\, Z(X_i)\ i = 1,2,3 \ldots, N \tag{5.30}$$

Where λ_i is the weight for the observation 2 at location X_i. In kriging, the weight λ_i are calculated by equation (5.31) so to make sure that $Z^*(X_0)$ is unbiased and optimal.

$$\begin{cases} \sum_{j=1}^{N} \lambda_i \gamma(X_i, X_j) + \mu = (X_i, X_0)\ i = 1,2,3 \dots, N \\ \sum_{j=1}^{N} \lambda_j = 1 \end{cases} \quad (5.31)$$

Where, μ is the langrage multiplier.

Inverse Square distance, which is a technique usually used in geohydrology can be used to interpolate the groundwater level data. The weights λ_i are inversely proportional to the square of distance from the estimation points as:

$$\lambda_i = \frac{\frac{1}{(d_{0i})^2}}{\sum_{i=0}^{n} \frac{1}{(d_{0i})^2}} \quad (5.32)$$

Where, d_{0i} is the distance between the sample point and the estimated point.

The above explains how interpolation is applied in groundwater. Even though only one method was elaborated, there are many other methods that are used for interpolation of groundwater as mentioned in the above sections. The key question to ask is does interpolation always give us the true reflection or representation of what is actually happening in reality? In most cases, it is not and therefore most interpolation efforts results in wrong information and therefore wrong interpretation of the system as will be shown in figure 7.

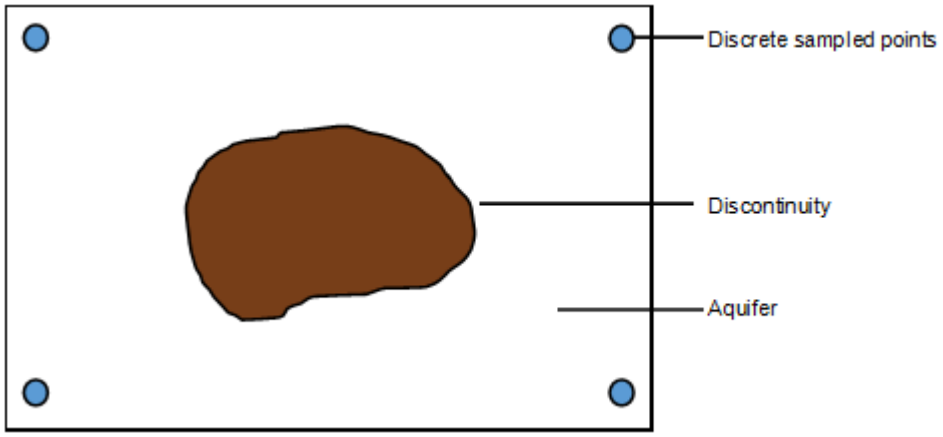

Figure 7: Aquifer system showing discrete sampling points and a discontinuity.

The figure above shows an aquifer system where measurements or sampling was done at discrete sampling points. Within the system, there is a discontinuity which can be an impermeable rock material. Based on the definition and properties of interpolation, we are made to understand that in order to interpolate a system accurately, there system needs to be continuous. In such a case where there is a discontinuity in an aquifer, one realizes that the normally used interpolation techniques that do not account for discontinuities in the system cannot be relied upon as they often will give wrong information about the system.

This rises a different question as to when can interpolation be used and when it cannot be applied? The following section helps us to understand the concept of multi-step interpolation concept which can be very helpful in dealing with problems which normal interpolation techniques cannot deal with.

5.4.1 Multi Step Interpolation Concept

Conceptually, every numerical method starts from an initial point and then takes a step forward in time. This helps to find the solution of the next point. This process carries on, step after step to map out the solution. Single step methods refer to only one previous point and its derivative to determine the current value. Such methods usually discard all previous information before taking another forward step. On the other hand, Multi-step methods keep and use information from all previous steps and do not remove or discard any information. Therefore, multi-step methods refer to several previous points and derivative values. The characteristics feature of one-step is that they need for computing y_{K+1} more than one of the previous approximations y_k, y_{k+1}.

5.4.1.1 Linear q-Step Method

Definition 1: A q step method with $q \geq 1$ is a numerical method for approximately solving:

$$y'(x) = f\big(x, y(x)\big), \quad y(x_0) = y_0 \tag{5.33}$$

$$y_{k+1} = \sum_{j=0}^{q-1} a_j\, y_{k-j}$$

$$+ h \sum_{j=0}^{q-1} bjf\left(x_{k-j}, y_{k-j}\right)$$

$$+ hb_{-1}\, f(x_{k+1}, y_{k+1}), K = q, q+1 \qquad (5.34)$$

With $q \geq 1, a_0, \ldots, a_{q-1}, b_{-1}, \ldots, b_{q-1} \in \mathbb{R}, a_{q-1} \neq 0\ or\ b_{q-1} \neq 0$. For $q = 1$, the method is called a one-step method. If $b_{-1} \neq 0$, then the linear q-step method becomes implicit, if not, it's an explicit method. This multi-step method requires initial q values. Equation (5.33) only provides the initial value y_0 and initial value y_1 has to be computed using the one-step method. The following initial value y_z can be derived using a one-step method or a multi-step method and the process continues to subsequent steps.

All initial values $y_i, i > 0$, are numerical assumptions. This setback can be accounted for in the error analysis stage.

5.4.1.2 Predictor Corrector Methods

The initial point of predictor corrector methods corresponds to the integral form of the initial value shown in equation (5.33).

$$y(x) = y_0 + \int_{x_0}^{x} f(t, y(t))\, dt \qquad (5.35)$$

Denote the solution at x by $y(x)$, then it holds that:

$$y(x) = y(x) + \int_{\underline{x}}^{x} f(t, y(t))\, dt \qquad (5.36)$$

Predictor corrector methods helps approximate the integral on the right-hand side of equation (5.36). However, there are two challenges:

- The dependency of the term in the integral on t is generally not known since the function $y(t)$ is unknown.
- Even if the dependency of the function in the integral on t is known, its practically impossible to find an analytical expression of the solution.

If we assume that the term in the integral of equation (5.36) is known, the derivation becomes similar to the derivation of the Newton-Cotes formulas of numerical quadrature. Following this sequence, the term in the integral of equation (5.36) is then replaced by a polynomial interpolant. Equidistant nodes are used in the construction of the polynomial:

$$x_i = x_0 + ih, \qquad i = 0,1, \ldots.$$

Let the boundaries of the integral be the nodes:

$x = x_{p-j}$, starting point with parameter j,

$x = x_{p+m}$, end point with parameter m,

Since $j, m, \in, \mathbb{N}_0$ parameters have not been determined, the interpolation polynomial $p(x)$ must satisfy the following parameters:

- The degree of $p_r(x)$ is lower than or equal to r.
- $p_r(x_i) = f(x_i, y(x_i))$ for $i = p, p-1, \ldots, p-r$.

Thus, x_p is the most right-hand side node for computing the interpolation polynomial. Lagrange (1736 – 1813) first proposed the solution of this interpolation problem:

$$p_r(x) = \sum_{i=0}^{r} f\left(x_{p-l}, y\left(x_{p-l}\right)\right) L_i(x)$$

With,

$$L_i(x) = \prod_{l=0, l\neq i}^{r} \frac{x - x_{p-l}}{x_{p-1} - x_{p-1}}, i = 0,1, \ldots, r.$$

Using equation (5.36), it follows that:

$$\begin{aligned} y_{p+m} &\approx y_{p-j} \\ &+ \sum_{i=0}^{r} f\left(x_{p-i}, y\left(x_{p-i}\right)\right) \int_{\underline{x}}^{x} L_i(t)\, dt \\ &= y_{p-j} + h \textstyle\int_{i=0}^{r} \beta_i f(x_{p-i}, y(x_{p-i})). \end{aligned} \tag{5.37}$$

With,

$$\beta_i = \frac{1}{h}\int_{\underline{x}}^{x} L_i(t)\,dt = \frac{1}{h}\int_{\underline{x}}^{x}\left(\prod_{l=0,l\neq i}^{r}\frac{t-x_{p-1}}{x_{p-i}-x_{p-1}}\right)dt$$

This method becomes linear. Using the substitution:

$$t = x_p + sh = x_0 + (p+s)h,$$

And the equidistant mesh yields:

$$\begin{aligned}\beta_i &= \frac{1}{h}\int_{-j}^{m}\left(\prod_{l=0,l\neq i}^{r}\frac{x_p+sh-x_{p-1}}{x_{p-i}-x_{p-1}}\right)h\,d_s \\ &= \int_{-j}^{m}\left(\prod_{l=0,l\neq i}^{r}\frac{ph+sh-ph+lh}{ph-ih-ph+lh}\right)ds \\ &= \int_{-j}^{m}\left(\prod_{l=0,l=i}^{r}\frac{s+l}{-i+l}\right)ds \end{aligned} \tag{5.38}$$

From the above, one can now get different methods depending on which parameters $(m, j\ and\ r)$ one chooses and by replacing $y(x_{p-i})$ in equation (5.35) with y_{p-i}.

5.4.1.2.1 Adams Bashforth Methods

The Adams-Bashforth method is given by parameters $m = 1,\ j = 0, and\ r = q-1$. The q-step Adams Bashforth method uses the nodes $x_{k+1} - q, \dots, x_k$ for computing the Lagrangian interpolation polynomial. These are q nodes and $p_q(x)$ is at most of degree $q-1$ (Lambers, 2011). This method has the following form:

$$y_{k+1} = y_K + h\sum_{i=0}^{q-1}\beta_i f(x_{k-i}, y_{k-i}) \tag{5.39}$$

With,

$$\beta_i = \int_0^1\left(\prod_{l=0,l\neq i}^{q-1}\frac{s+1}{-i+1}\right)ds \tag{5.40}$$

Where $q = 1$, the term in the integral in equation (5.36) is replaced by a constant interpolation polynomial with the node $x_k, f(x_k, y_k))$ This gives:

$$y_{k+1} = y_k + h\left(\int_0^1 ds\right) f(x_k, y_k)$$

$$= y_k + hf(x_k, y_k) \tag{5.41}$$

From the above, the explicit Euler method is obtained. Furthermore, if $q = 2$, the term in the integral is estimated by linear polynomial with the nodes $x_{k-1}, f(x_{k-1}, y_{k-1}))$ and $x_k, f(x_k, y_k))$. Equation (5.39) and (5.40) yields:

$$y_{k+1} = y_k + h\int_0^1 \left(\frac{s+1}{1}\right) dsf(x_k, y_k)$$

$$+ h\int_0^1 \left(\frac{s}{-1}\right) dsf(x_{k-1}, y_{k-1})$$

$$y_k + h = \left[\frac{3}{2}f(x_k, y_k) - \frac{1}{2}f(x_{k-1}, y_{k-1})\right]$$

$$= y_k + \frac{h}{2}[3f(x_k, y_k) - f(x_{k-1}, y_{k-1})] \tag{5.42}$$

5.4.1.2.2 Adams-Moulton Method

This method uses the following choice of parameters; $m = 0,\ j = 1, and\ r = q$. Therefore, it follows that,

$$\beta_i = \int_{-1}^{0}\left(\prod_{l=0, l\neq i}^{q} \frac{s+l}{-i+l}\right) ds \tag{5.43}$$

Together with,

$$y_k = y_{k-1} + h\sum_{i=0}^{q} \beta_i f(x_{k+1-i}, y_{k+1-i}) \tag{5.44}$$

Or, by changing the index,

$$y_{k+1} = y_k + h\sum_{i=0}^{q} \beta_i\, f(x_{k+1-i}, y_{k+1-i}) \tag{5.45}$$

Nodes are given by $x_{k+1-q}, \ldots, x_k, x_{k+1}$. Unlike the Adam-Bashforth method, Adam-Moulton methods are implicit methods (Lambers, 2011).

Where $q = 0$, the term in the integral is replaced by constant interpolation polynomial with the node at $x_{k+1}, f(x_{k+1}, y_{k+1}))$.

This yield:

$$\begin{aligned} y_{k+1} &= y_k + h\left(\int_{-1}^{0} ds\right) f(x_{k+1}, y_{k+1}) \\ &= y_k + hf(x_{k+1}, y_{k+1} \end{aligned} \tag{5.46}$$

The above gives implicit Euler method.

When $q = 1$, we can use a linear interpolation polynomial with the points $x_k, f(x_k, y_k))$ and $(x_{k+1}, f(x_{k+1}, y_{k+1}))$. We get:

$$\begin{aligned} y_{k+1} = y_k + h[&\left(\int_{-1}^{0} \frac{s+1}{1} ds\right) f(x_{k+1}, y_{k+1}) \\ &+ \left(\int_{-1}^{0} \frac{s}{-1} ds\right) f(x_k, y_k))] \\ y_k + h\,[&\frac{1}{2} f(x_{k+1}, y_{k+1}) + f(x_k, y_k))] \\ = y_k + &\frac{h}{2}[f(x_{k+1}, y_{k+1}) + f(x_k, y_k))]. \end{aligned} \tag{5.47}$$

The method used is referred to as the trapezoidal rule.

5.4.1.2.3 Nylstroom Methods

This method was first introduced by Evert J. Nystroom (1895 – 1960). This type of method is obtained by using $m = 1,\ j = 1, and\ r = q - 1$. Nystroom methods have the following form:

$$y_{k+1} = y_{k-1} + h \sum_{i=0}^{q-1} \beta_i f(x_{k-i}, y_{k-i}) \tag{5.48}$$

Together with,

$$\beta_i = \int_{-1}^{1} \left(\prod_{l=0, l \neq i}^{q-1} \frac{s+1}{-i+l} \right) ds \tag{5.49}$$

Nylstroom methods are explicit and one method uses the following q nodes $x_{k+1-q}, \ldots, x_k$.

When $q = 1$, the method gives:

$$\begin{aligned} y_{k+1} &= y_{k-1} + h \left(\int_{-1}^{1} ds \right) f(x_k, y_k) \\ &= y_{k-1} + 2hf(x_k, y_k) \end{aligned} \tag{5.50}$$

5.4.1.2.4 Milne Methods

Milne methods are defined by $m = 0,\ j = 2, and\ r = q$. Using a transform of the index, they have the following form:

$$y_{k+1} = y_{k+1} + h \sum_{i=0}^{q} \beta_i f(x_{k+1-i}, y_{k+1-i}) \tag{5.51}$$

Together with,

$$\beta_i = \int_{-2}^{0} \left(\prod_{l=0, l \neq i}^{q} \frac{s+l}{-1+l} \right) ds \tag{5.52}$$

Milne methods are implicit.

When implicit methods are required to be used, we have to solve a non-linear equation in each node x_{k+1}. This step has to be performed with repetition to achieve good efficiency using the method. An explicit multi-step method can be used to get a good initial iterate. For this reason, explicit multi-step methods are called predictor methods and implicit multi-step methods are called corrector methods. Combining the two methods results in a predictor-corrector method (Lambers, 2011).

5.4.1.2.5 Nordsieck Methods

This method transforms multi-step methods in a one step form. Instead of,

$$y_k, \dots, y_{k-q+1}, f(x_k, y_k), \dots, f(x_{k-q+1}, y_{k-q+1}),$$

The method uses the values,

$$y_k, y'(x_k), y''(x_k), \dots, y^{(q)}(x_k),$$

The Nordsieck form applies a step length control as It is known from one step methods. This is one advantage of the Nordsieck method. Without this control, multi-step methods would be complicated.

CHAPTER SIX: NUMERICAL SIMULATIONS

In this section, we present numerical simulations of the suggested equation for different values of scale factor. The numerical simulations are obtained using some theoretical values of aquifers parameters. The new parameter added in this work help us to see how the cell size or scale factor influences the change in drawdown. This is the main important parameter that was removed by Theis to obtain a simpler groundwater flow equation that does not include the scale factor. We thus depict the numerical simulations in figure 8, 9, 10, 11, 12, 13, 14, 15, 16 and 17 for different values of scale factor.

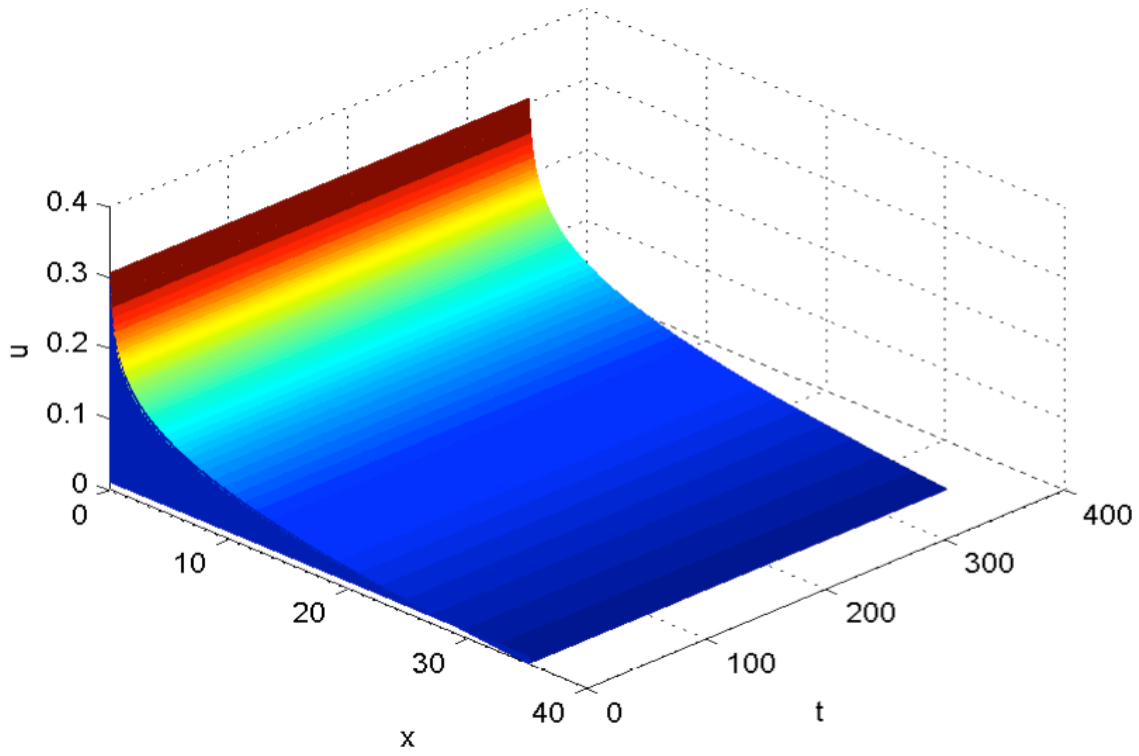

Figure 8: The numerical simulation for scale factor equals 0.08.

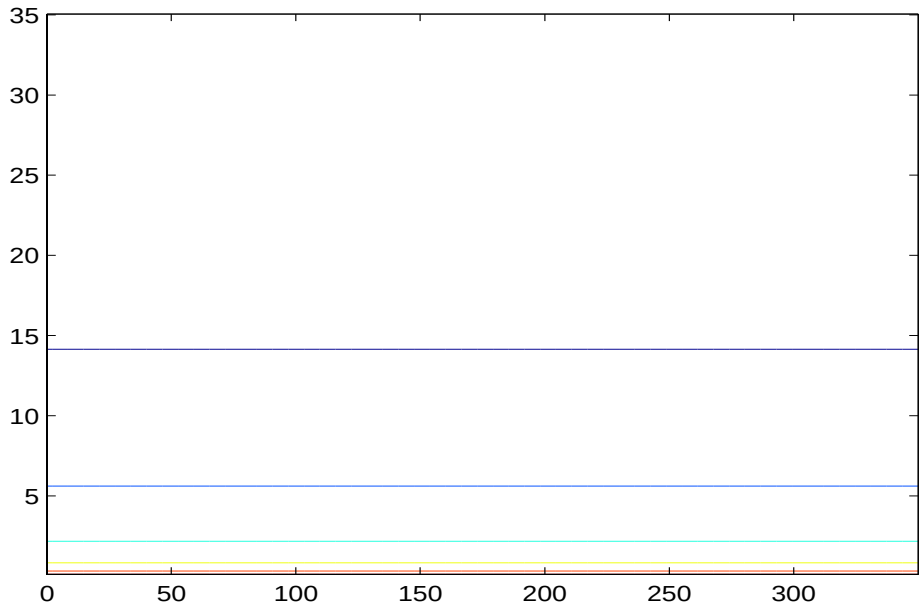

Figure 9: Contour plot of numerical simulation for scale factor 0.08.

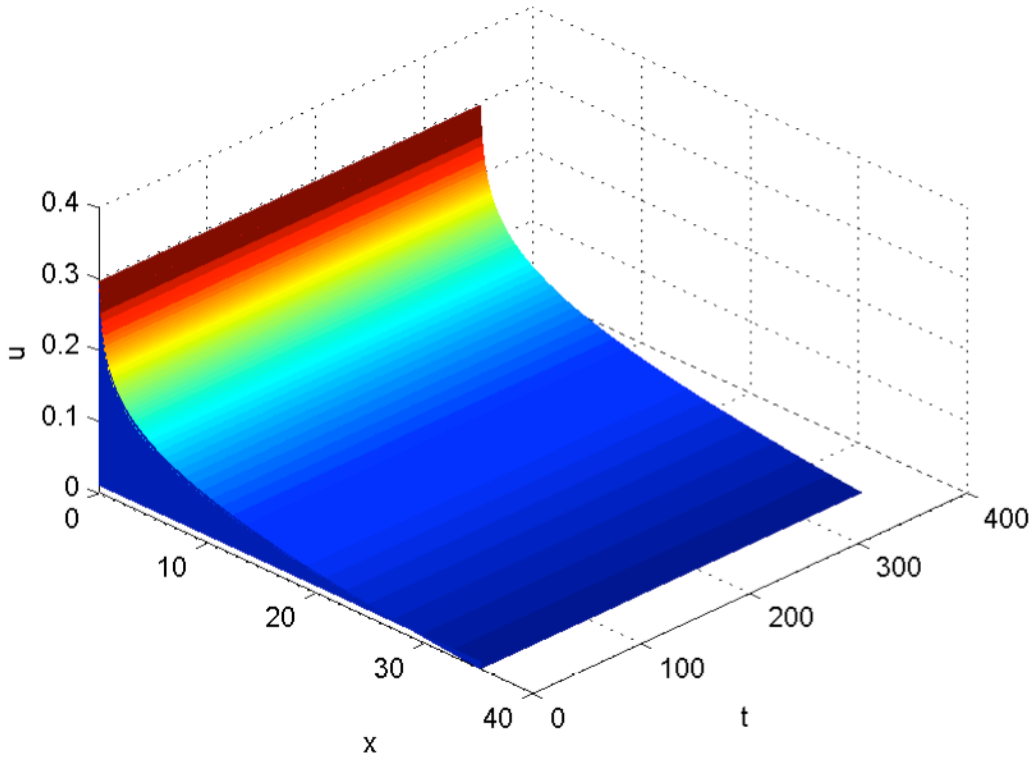

Figure 10: Numerical simulation for scale factor 0.07.

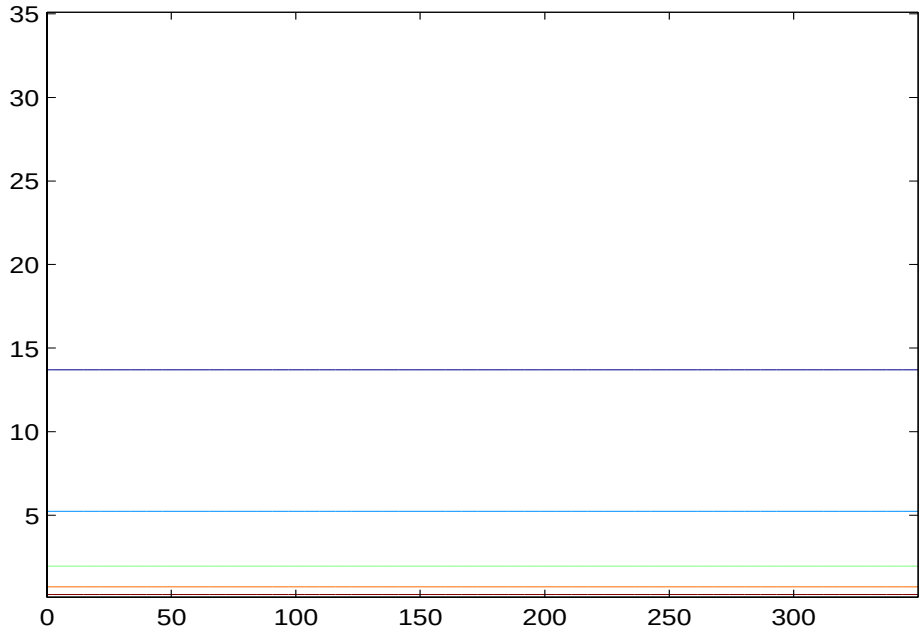

Figure 11: Contour plot of numerical simulation for scale factor 0.07.

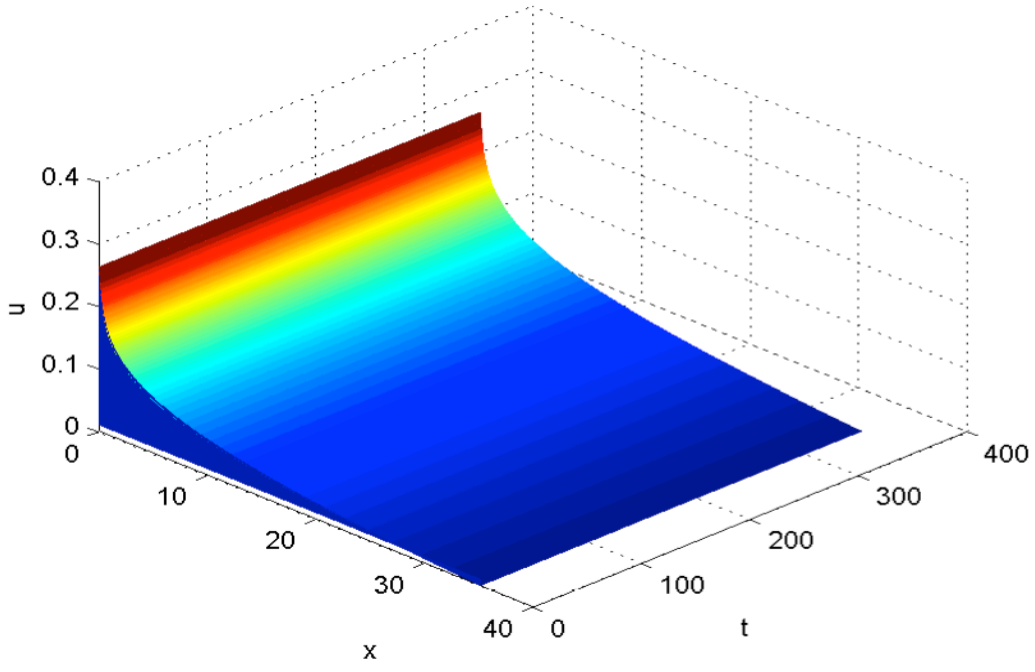

Figure 12: Numerical simulation for scale factor equals 0.05.

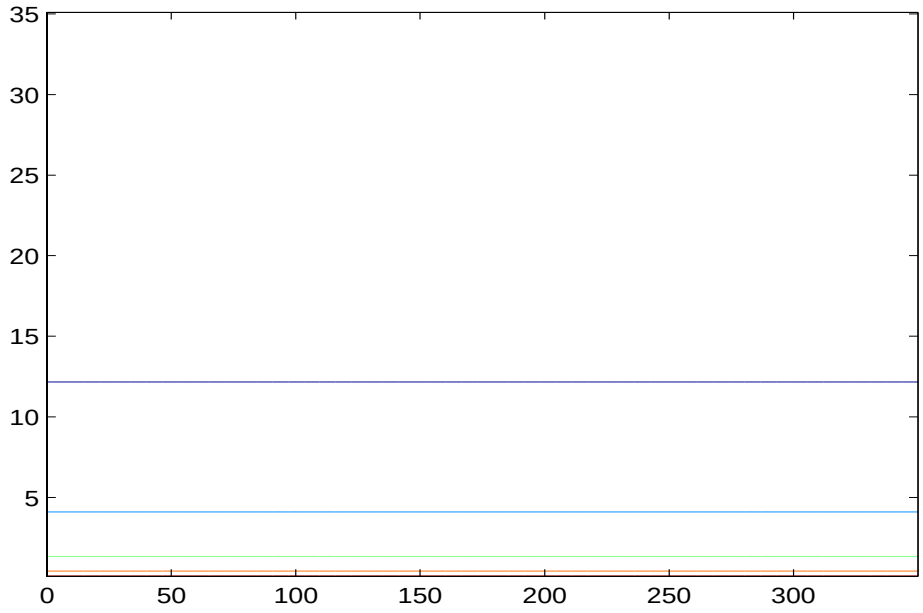

Figure 13: Contour plot of the numerical simulation for scale factor equals 0.05.

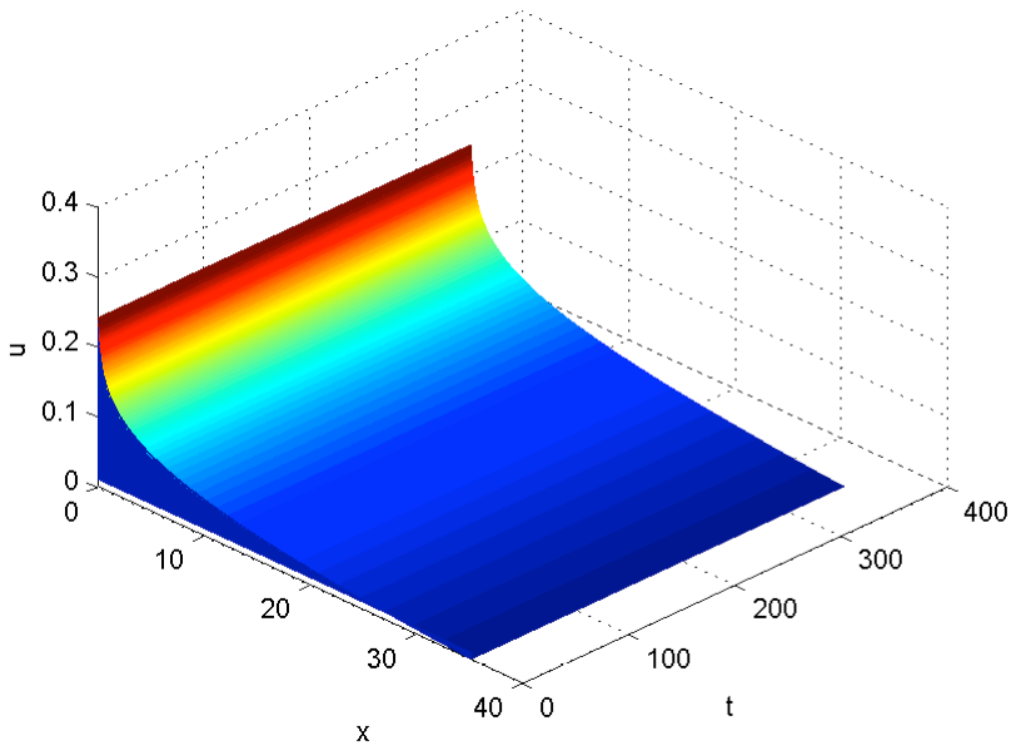

Figure 14: Numerical simulation for scale factor equals 0.02.

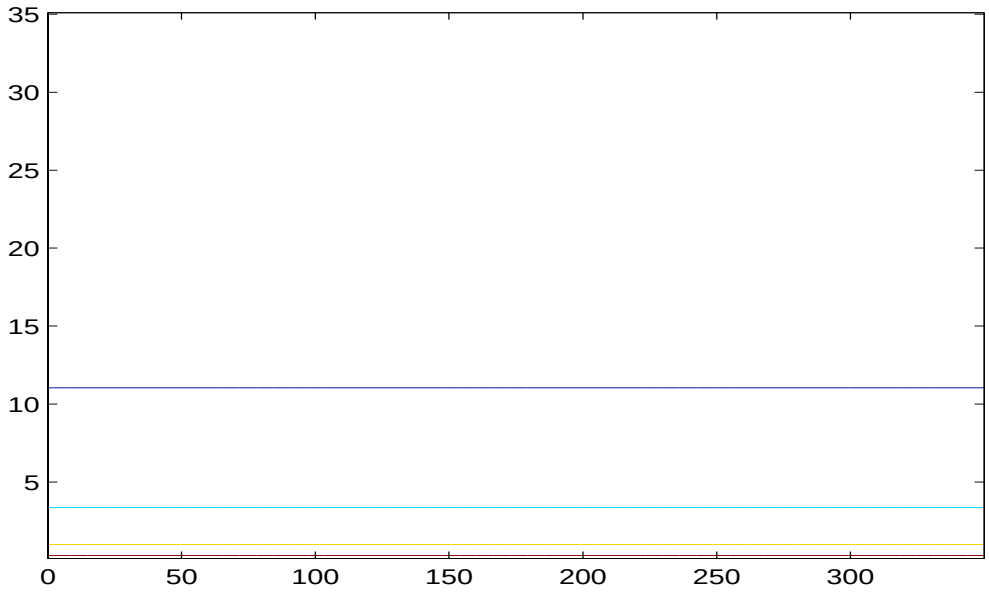

Figure 15: Contour plot of numerical simulation for scale factor equals 0.02.

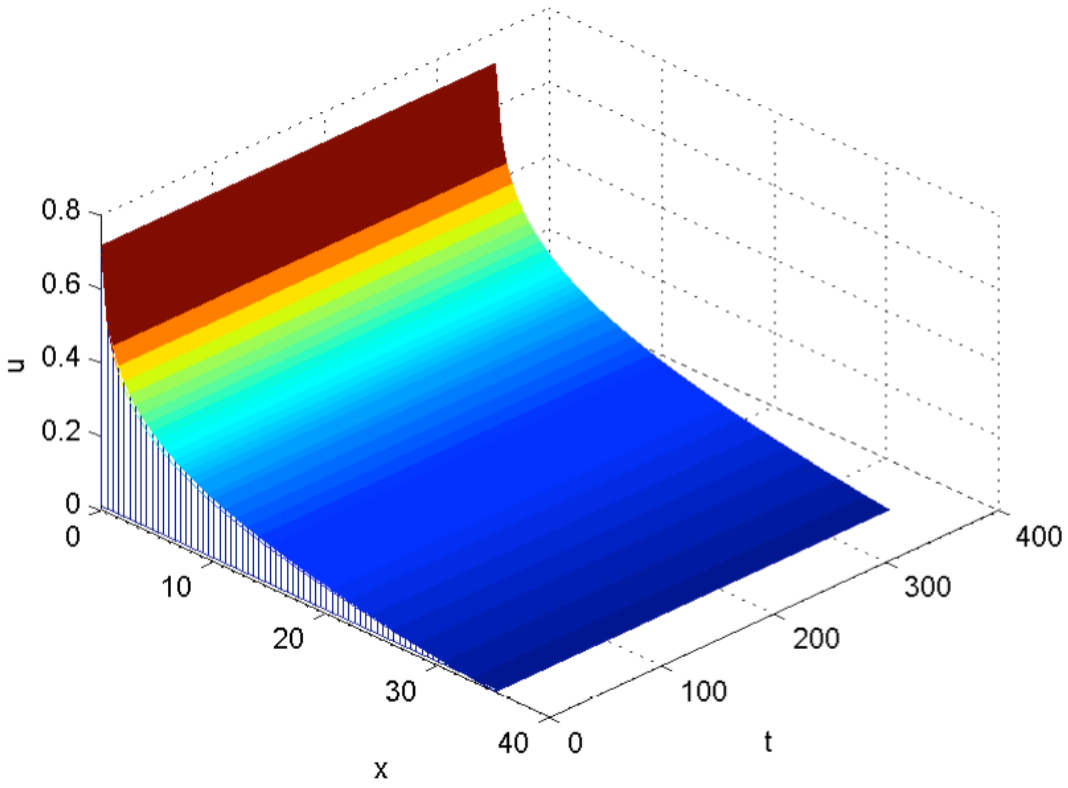

Figure 16: Numerical simulation for scale factor equals 0.5.

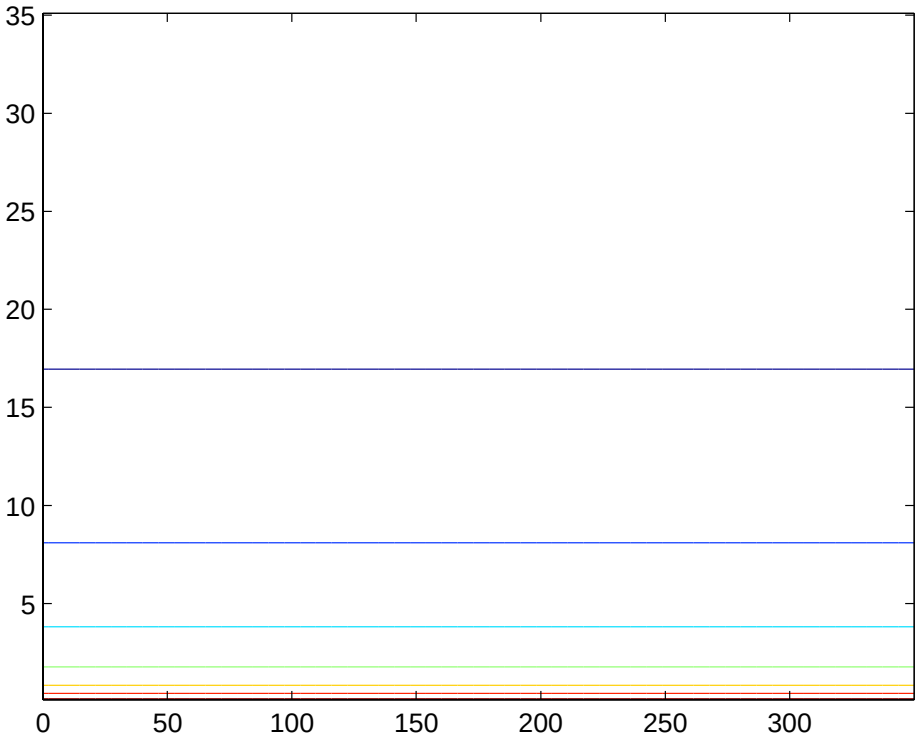

Figure 17: Contour plot of numerical simulation for scale factor equals 0.5.

The above simulations show that the new physical parameter included in our newly developed equation play an important role. Based on the numerical simulations and contour plots, we observe that the change in drawdown depend on this physical parameter. As stated in the introduction, the new physical parameter is the scaling factor which Theis removed in his equation. Theis equation does not take into account the scaling factor. This physical parameter helps us to observe the gradual change in drawdown without overestimating or underestimating the change. The smaller the size of the cell, the better we see the change in drawdown but if the cell is too small, we can underestimate the drawdown. If the cell is too large, we tend to overestimate the drawdown.

Figure 8 shows a scale factor of 0.08 and we observe that the drawdown in the numerical simulation starts above $0.3u$ and gradually decreases with time. The contour plot in figure 9 also shows a gradual change in drawdown, which supports what has been depicted by the numerical simulation.

As the scaling factor is decreased as shown in figure 10, 11, 12, 13, 14, 15, 16 and 17, we observe that even the rate of drawdown changes. This trend can be observed in all the numerical simulations and contour plots. It can be seen that increasing or decreasing of the scaling factor has a direct impact on the change of drawdown.

CONCLUSION

The main aim of this research was to develop the exact groundwater model within a confined aquifer. The aim was to also extend the limitation of Theis equation that does not entirely give a true representation of what actually happens in reality. In addressing this aim, an exact groundwater flow equation in confined aquifer was derived. The equation was proven that it has unique solution. A new numerical scheme was developed using the Mellin transform, Adam Bashforth method and inverse Mellin transform. The exact groundwater flow model within confined aquifers was simulated using the newly developed numerical scheme. The exact solution for groundwater flow equation for a confined aquifer was derived using the Boltzmann transform. In conclusion, the newly developed groundwater flow equation has a new physical parameter. It can be concluded that the new physical parameter has an important role. The new physical parameter is the scaling factor. It can also be concluded that this is also the parameter which was removed by Theis so as to get a simple model. From the numerical simulations and contour plots, we observed that the change in drawdown depends on this physical parameter. The smaller the size of the cell, the better we observe the change in drawdown but it must also be noted that if the cell size is too small, the drawdown can be underestimated. However, if the cell size is too large, the change in drawdown tends to be overestimated. In conclusion, our model differs from Theis due to the introduction of a physical parameter called the scaling factor. The cell size from one step to another is different from Theis.

In conclusion, we also proposed a new way of applying interpolation in groundwater. Multi-step interpolation technique can be very helpful with challenges or problems which normal interpolation techniques cannot deal with. For instance, this type of interpolation technique can account for discontinuities that may occur within the system underground such as dykes and sills.

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ABSTRACT

The main aim of this research was to develop the exact groundwater flow model within a confined aquifer. We argued that, the Theis groundwater flow model is an approximation of the real formulation of the model as he removed some components of the equation to have a simple model. Initially, we derived an exact groundwater flow equation for a confined aquifer so as to include all high order terms that was removed by Theis and also to take into account the assumptions that was used during the derivation of the groundwater flow by Theis. Thereafter, we proved that the new groundwater flow equation has unique solution. We then derived a new numerical scheme for singular partial differential equation that combines the Mellin transform and the Lagrange approximation of a continuous function. The Mellin transform was used to remove the singularity in the newly developed exact groundwater flow equation for a confined aquifer. The equation became ordinary, wherein we used the Adam Bashforth method to the ordinary differential equation in Mellin space. The inverse of Mellin was then used to get the exact numerical scheme in real space. The derivation of the exact solution of groundwater flow equation for a confined aquifer was derived and shown using the Boltzmann transform. We presented the stability analysis of the new numerical scheme using the von Neumann method. We also discussed the application of data in groundwater modelling. We argued that, most methods used in the collection of data lead to incorrect representation of reality or the system under investigation. The application of mathematics to aid in data processing was also suggested. Various interpolation methods used in groundwater were also discussed. We proposed the concept of Multi-step interpolation technique. Lastly, numerical simulations using experimental field data was presented. Our solution was compared to Theis. Our simulations show the importance of scaling factor which was removed from the Theis groundwater flow equation. The simulations also show that the change in drawdown depend on the scaling factor.

Keywords: Groundwater flow equation; Stability; Mellin transform; Confined aquifer; Numerical scheme; Singular partial differential equation.