DETERMINISTIC AND STOCHASTIC ANALYSIS OF GROUNDWATER IN UNCONFINED AQUIFER MODEL

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DECLARATION

I hereby declare that this dissertation “Deterministic and Stochastic analysis of groundwater in unconfined aquifer model”, is of my own work. The dissertation was carried out at the Institute for Groundwater studies, University of the Free State, Bloemfontein, under the supervision of Professor Abdon Atangana. I earnestly declare that, to the best of my knowledge, no part of this dissertation was previously submitted for the requirements of a degree, diploma or any other title of recognition at any institution. All sources used for this compilation have been fully acknowledged in the reference list.

With that said, I cede copyright of this dissertation in favour of the University of the Free State.

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Ramakatsa, D.G. and Atangana, A.; Deterministic and Stochastic analysis of groundwater in unconfined aquifer model

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ABSTRACT

In several developed countries, groundwater has been recognised as one of the most important natural source of fresh water. It can now be understood why many researchers from all corners from applied science have devoted their attention in developing new methods, models that could be used to monitor and understand the movement of this water within subsurface. The literature nowadays revealed different type of geological formations, including confined, leaky and unconfined aquifers. The movement of water within these three aquifers cannot be captured using the same mathematical models. The Theis model was introduced to capture flow within a confined aquifer, while the Hantush model was suggested to predict the flow within leaky aquifer, these two partial differential equations cannot account for the flow within an unconfined aquifer, and more precisely they are linear equations. To capture flow within an unconfined aquifer, a new mathematical equation was suggested and happens to be integro-differential type. The study of this model is not popular maybe due to the complexity of the mathematical setting. In this dissertation, we considered the model of groundwater flowing within an unconfined aquifer. We derived the conditions under which the exact solution can be obtained. We suggested numerical solutions using different schemes including forward Euler, Crank-Nicholson and Atangana-Batogna schemes. For each of them, we presented detailed study underpinning the stability of the used scheme. To conclude, we suggested a new numerical scheme that combines the fundamental theorem of calculus, Adams-Bashforth and the trapezoidal rule. The method is a new door for investigation in the field of modelling as it is highly accurate and efficient. In addition to this, we argued that differential equations with constant coefficient cannot capture complexities with statistical setting, to solve this problem in case; we converted all parameters included in our equation into distribution functions. The new model was also solved numerically. Lastly, we present numerical simulations from a software package called MATLAB, using normal and statistical data.

Keywords: Unconfined aquifer, density distributions, numerical analysis, stability analysis.

LIST OF GREEK NOTATIONS

α	alpha
β	beta
τ	tau
∂	partial differential
δ	delta
φ	phi
Δ	Delta
θ	theta
ϕ	phi
Φ	Phi
σ	sigma
Σ	Sigma
μ	mu
λ	lambda
ω	omega
ξ	xi

ABBREVIATIONS AND NOTATIONS

T	Transmissivity
t	Time
S	Storativity
S_s	Specific storage
S_y	Specific yield
K	Hydraulic conductivity
h	Hydraulic head
r	Radial distance
Q	Discharge
q	Darcy flux
n	Porosity
s	Drawdown
v	Velocity
f	Function
b	Aquifer thickness

Table of Contents

LIST OF FIGURES

CHAPTER ONE: INTRODUCTION

1.1 Background

Groundwater is the water preserved in permeable media such as ground pore spaces or rock formations under the surface of the earth. Groundwater flow is the motion of water in the underground porous media. An aquifer is regarded as a geological formation or stratum that comprises groundwater and enables large amounts of groundwater to pass through it under normal ground conditions. (Neuman.,1972, 1974), (Dagan and Kroszynski.,1975). The groundwater behaviour during the groundwater movement process through an aquifer system depends on the characteristics of the water itself and the medium in which it flows. Groundwater models such as deterministic mathematical models and stochastic models are most designed to represent the flow mechanisms in groundwater systems to understand groundwater behaviour. The function of groundwater flow modelling is to estimate flow speeds or head forecasts. However, speed estimates are generally based on hydraulic head differences and are therefore much more sensitive to numerical modelling errors than hydraulic head estimates alone. Meaningful transport predictions often involve the calculation of the speed range on a fine spatial grid. Analytical solutions therefore have a certain advantage over numerical processes. (Neuman.,1972,1974). Deterministic and stochastic groundwater mathematical models are usually used through partial differential equations to simulate flow and transport processes in aquifer systems. A stochastic model is a predicament in which there is uncertainty. In other words, this is a model for a process that is random. The word stochastic comes from the Greek word "*stokhazesthai*", which means aiming or speculating. In the real world, uncertainty is a part of the norm; therefore, a stochastic model can depict literally anything. On the contrary, the deterministic model is one that predicts the output with 100% certainty. Deterministic models always have an equation set that accurately describes the system inputs and outputs. This means that stochastic models will probably yield different results each time the model runs.

1.2 Problem statement

The movement of water within a confined, unconfined or leaky aquifer cannot be captured using the same mathematical models. The Theis model was introduced to capture flow within a confined aquifer, while the Hantush model was suggested to predict the flow within leaky aquifer, these two partial differential equations cannot account for the flow within an unconfined aquifer, and more precisely they are linear equations. For instance, The Theis (1935) equation for groundwater flow happens to be one of the elemental keys for solving groundwater related problems in a confined aquifer system. Thus, it serves as one of the primary solutions for groundwater flow in the deterministic mathematical models. Theis (1935) equation was attained based on certain assumptions. The assumptions state that the aquifer should be homogeneous, with uniform thickness, isotropic, has infinite aerial extend and is pumped at a constant discharge rate. However, in reality, the opposite is true in that the aquifer is usually heterogeneous, anisotropic, pumped at different discharge rates and has finite aerial extend resulting from impermeable boundaries. To capture flow within an unconfined aquifer, a new stochastic mathematical equation was suggested and happens to be integro-differential type. The study of this model is not popular maybe due to the complexity of the mathematical setting. In this dissertation, we considered the model of groundwater flowing within an unconfined aquifer. We derived the conditions under which the exact solution can be obtained. We suggested numerical solutions using different schemes including forward Euler, Crank-Nicholson and Atangana-Batogna schemes. For each of them, we presented detailed study underpinning the stability of the used scheme. To conclude, we suggested a new numerical scheme that combines the fundamental theorem of calculus, Adams-Bashforth and the trapezoidal rule.

1.3 Unconfined aquifer

A groundwater aquifer is referred to as unconfined when its upper surface (water table) through permeable material is open to the atmosphere. In contrast to a confined aquifer, the water table in an unconfined aquifer system does not have an overly impermeable rock layer that separates it from the upper atmosphere. Water table aquifers are generally shallower to the surface of the Earth than confined aquifers and are affected sooner by drought than in confined aquifers. (Kroszynski and Dagan.,1975). Figure 1 depicts a cross section through different aquifers, including the unconfined aquifer.

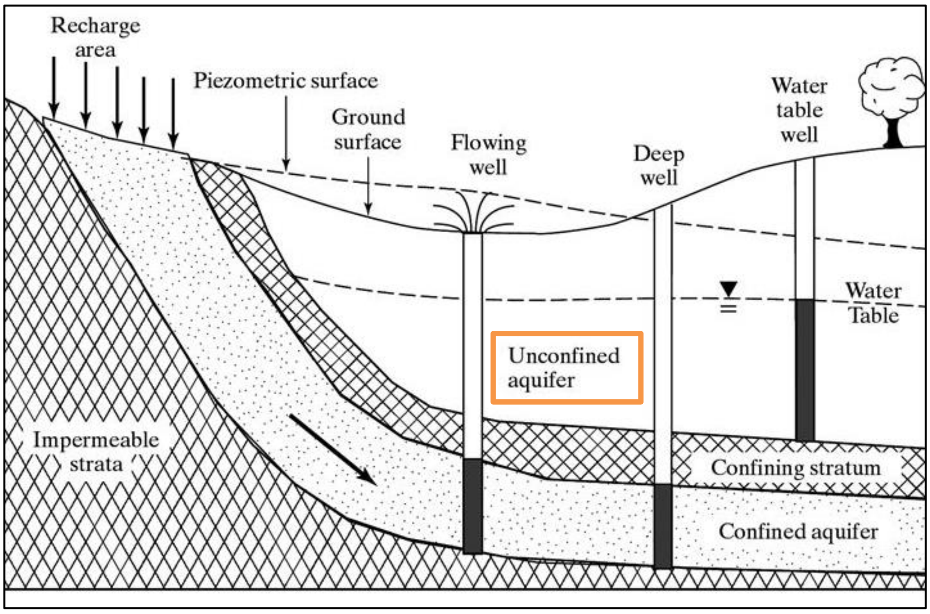

Figure 1: Schematic cross section illustrating an unconfined aquifer (Kroszynski and Dagan, 1975).

1.4 Deterministic approach

Deterministic mathematical models usually simulate flow and transportation processes in groundwater systems using partial differential equations (Bear., 1972; Anderson and Woessner., 1992; Konikow., 2001). Presuming the groundwater flow is a time-reliant fundamental problem, full expressions of the deterministic mathematical models include statements of equations, initial and boundary conditions. Mathematical deterministic models can be easily resolved either analytically or numerically. Analytical solutions however require generally highly idealized and detailed parameters and boundaries.

The governing equations are mathematical relations that describe groundwater movement approximations via aquifer mechanisms. They can be derived directly from different concepts of groundwater systems by incorporating water mass balance mathematically with Darcy's law (Darcy.,1856). There are two different concepts of groundwater systems: (1) the viewpoint of the aquifer and (2) the viewpoint of the flow system. The view of aquifers is based on concepts of confined and unconfined aquifers (Anderson and Woessner.,1992). A general form of the governing equation in a confined aquifer can be expressed as:

$$\frac{\partial}{\partial x}\left(T_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_y\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}-R+L \quad (1.1)$$

Where h is the hydraulic head. T_x and T_y are horizontal transmissivity components. S represents the coefficient of storage. R depicts a sink/ source phrase that is identified as intrinsically valuable for recharge. L represents leakage in a confined bed (Anderson and Woessner.,1992).

In an unconfined aquifer, the components of transmissivity that are practically assumed, T_x and T_y, in Equation (1.1) are substituted by $T_x = K_x h$ and $T_y = K_y h$, respectively, and the L component which represents leakage in Equation (1.1) is equivalent to zero. This result in a nonlinear governing equation, also referred to as Boussinesq equation (Bear.,1972; Anderson and Woessner.,1992), representing an unconfined aquifer flow as:

$$\frac{\partial}{\partial x}\left(K_x h\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}K_y h\left(\frac{\partial h}{\partial y}\right)=S_y\frac{\partial h}{\partial t}-R \quad (1.2)$$

Where h, represents the saturated thickness in an unconfined aquifer, K_x and K_y are tensor conductivity horizontal components. S_y is an unconfined aquifer's specific output. The flow mechanism view point relates to three-dimensional head distribution, hydraulic conductivity and groundwater storage properties. It enables vertical and horizontal flow components to be analysed and therefore enables evaluations of two-dimensional or three-dimensional groundwater flow. A standard form of the regulatory equation for the flow system is:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}-R \quad (1.3)$$

where K_x is the vertical conductivity tensor component. S_s represents the specific storage. R represents a sink/source phrase denoted as the system input volume per unit volume of aquifer per unit time (Anderson and Woessner.,1992). Since groundwater flow motions are described in general, the governing equations do not produce any information on the characteristics of unique groundwater flow instances. In order to obtain solutions for special cases, the limits and initial conditions must also be specified together with the relevant equations. The boundary conditions represent mathematical statements that specify the dependent variable or derivative of the dependent variable at the boundary of problems relating to groundwater. (Anderson and Woessner.,1992).

1.5 Stochastic approach

Historically, groundwater movement in aquifers was deterministically modelled, which assumes that the information required in the modelling, such as aquifer parameters and boundary conditions, should be known with certainty. Therefore, a unique solution correlated with the set of deterministic conditions can be obtained. Hydrological events are better described in reality as random encounters. The boundary conditions, such as the river stage, can be uncertain or even unknown, more especially when future predictions are to be made. The aquifer parameters, such as hydraulic conductivity, transmissivity and storativity are also random variables because of the lack of information and/or the underlying complexity of the geologic process. Therefore, groundwater flow is more realistically modelled using the stochastic approach.

The hydraulic head distribution equation in a transient two-dimensional aquifer system with spatially randomly chosen transmissivity and spatio-temporally recharge is expressed as:

$$\frac{\partial}{\partial_{xi}}\left[T(x)\frac{\partial H}{\partial_{xi}}\right] + R(x,t) = S_y\frac{\partial H}{\partial t} \quad (1.4)$$

Where:

$x = (x_{1,}x_2)$ represents a vector point in the horizontal plane, T(x) represents transmissivity at a specific location x, R(x,t) denotes transient recharge at a particular time t and location x. The transient hydraulic head is represented by $H(x,t)$ at a specific time t and location x, S_y represents the specific yield, which is the volume of water produced per unit area per unit head decline, which serves as a known constant.

Pore water velocity vector for two-dimensional transient flow is:

$$V_i(x,t) = \frac{T(x)}{bn}\frac{\partial H(x,t)}{\partial_{xi}} \quad (1.5)$$

i=1.2

Where in $V_i(x,t)$ at vector location x and time t is the pore velocity, $T(x)$ is the transmissivity, b is the thickness of the aquifer, and n represents the porosity. Here, both the thickness of the aquifer and porosity are generally known to be constants.

The figure below shows two different model types: the deterministic, by which the output depends entirely on the initial conditions and the parameter values. The stochastic model, on the contrary, has certain randomness.

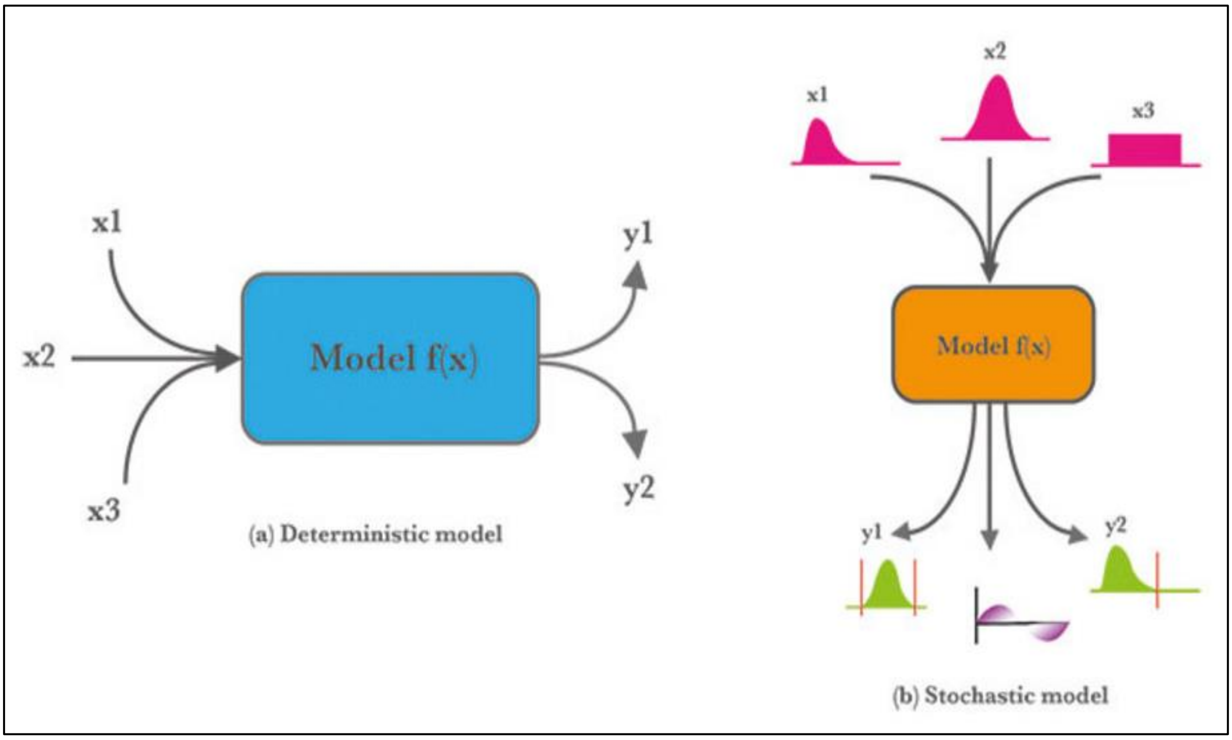

Figure 2: Representation of the two models: Deterministic and Stochastic (Gallage et al, 2013).

1.6 Numerical approximation

Boulton (1954b) extended the transient confined theory of Theis to include the effect of delayed yields in unconfined aquifers due to the movement of the water table. The solutions proposed by Boulton (1954b;1963) reproduce the unconfined time-drawing curve in all three segments. In its formulation of delayed yields, it assumed that as the water table falls, water is gradually released from storage (drainage) rather than instantly, as in the Boulton (1954a) and Dagan (1967) free-surface solutions. This approach resulted in an integrated differential flow equation in terms of average drawdown s^* as:

$$\frac{\partial^2 s^*}{\partial r^2} + \frac{1}{r}\frac{\partial s^*}{\partial r} = \left[\frac{S}{T}\frac{\partial s^*}{\partial t}\right] + \left\{\alpha S_y \int_0^t \frac{\partial s^*}{\partial \tau} e^{-\alpha(t-\tau)} d\tau\right\} \qquad \textbf{(}1.6)$$

Boulton linearized by denoting T a constant value. The phrase in square brackets is instantaneous confined storage, the phrase in braces represents a convolution integral which represents the storage that has been released steadily since the pumping started due to the decline of the water table. Boulton (1963) showed that the time when delayed yield effects are negligible is equivalent to α, leading to the term referred to as “the delay index”.(Prickett.,1965)

Prickett (1965) used this principle and developed an empirical relationship between the delay index and the physical aquifer properties by analysing large amounts of field drawdown data using Boulton 's (1963) solution. Prickett (1965) implemented an estimation methodology for S, S_y, K and α of unconfined aquifers by analysing pumping tests using the Boulton (1963) solution.

Although Boulton's model could replicate all three segments of the time-drawing curve in an unconfined aquifer, the physical mechanism of the delayed yield process was not explained by the non-physical nature of the "delay index" in the Boulton (1963) solution. Streltsova (1972a) invented an estimated solution for the water table decline and the complete penetration of pumping and observation wells. Like Boulton (1954b), Streltsova (1972a) represented the water table as a sharp material boundary and wrote the two-dimensional flow equation with average depth $as\ \partial^2$.

$$\frac{\partial^2 s^*}{\partial r^2} + \frac{1}{r}\frac{\partial s^*}{\partial r} = \frac{S}{T}\left(\frac{\partial s^*}{\partial t} - \frac{\partial \xi}{\partial t}\right) \tag{1.7}$$

The rate of decline in the water table was then presumed to be linearly proportional to the difference between and the vertically averaged head, $b - s^*$ and the elevation ξ of the water table.

$$\frac{\partial \xi}{\partial t} = \frac{K_z}{S_y b_z}(s^* - b + \xi\ ) \tag{1.8}$$

Where $bz = \frac{b}{3}$, represent the effective thickness of the aquifer over which the water table is recharged to the deep aquifer. Equation (1.8) can be seen as an estimate to Boulton (1954a) and Dagan (1967)'s zero-order linearized free-surface boundary condition. Streltsova considered the initial condition of $\xi(r, t = 0) = b$ making use of similar boundary condition at the pumping well and the outer boundary $r \to \infty$ of Theis (1935) and Boulton (1963), respectively. The solution is Equation (1.7) (Streltsov.,1972b)

$$\frac{\partial \xi}{\partial t} = -\boldsymbol{\alpha_T}\int_{\mathbf{0}}^{\boldsymbol{t}} \boldsymbol{e}^{-\alpha_T(t-r)}\frac{\boldsymbol{\partial s^*}}{\boldsymbol{\partial \tau}}\boldsymbol{d_\tau} \tag{1.9}$$

Where $\boldsymbol{\alpha_T} = K_z/(S_y bz)$. The substitution of equation (1.9) into (1.8) generates solution (1.6) Boulton (1954b, 1963); both solutions are roughly equal. The delayed yield theory of Boulton (such as that of Streltsova) doesn't at all account for water flow in unsaturated areas but treats water table as a material boundary moving vertically downwards under gravitational influence. Streltsova (1973) used raw data gathered by Meyer (1962) to show unsaturated flow of water, which had virtually no effect on the delayed process observed. Although Streltsova's solution linked the delay index of Boulton to physical aquifer properties, it later became a function of r.(Neuman.,1975; Herrera et al.,1978).

Boulton and Streltsova 's delayed yield solutions do not account for vertical flow in an unconfined aquifer by simplifying assumptions. These solutions cannot be broadened to account for partially penetrating pumping and observation wells. The pumping test carried out by Prickett near Lawrenceville, Illinois (Prickett., 1965) later depicted that specific storage in unconfined aquifers could be much higher than the observed values in confined aquifers–likely due to trapped air bubbles or aggregated shallow sediments. The elastic characteristics of unconfined aquifers are obviously too crucial to be ignored.

The models of Boulton (1954b; 1963) experienced conceptual difficulties outlining the physical mechanism of full release of water from storage in unconfined aquifers. Neuman (1972) described a physically focused mathematical model that regarded the unconfined aquifer as compressible (such as Boulton (1954b, 1963) and Streltsova (1972a, b)) as well as water table as a moving boundary (such as Boulton (1954a) and Dagan (1967). In Neuman's delayed response to the aquifer, triggered by the liberation of the physical water table, he implemented replacing the phrase "delayed yield" with "delayed water table response".

The Laplace equation of Boulton (1954a) and Dagan (1967) was replaced by the diffusion equation. Neuman (1972); it is denoted as:

$$\frac{\partial^2 s_D}{\partial {r^2}_D} + \frac{1}{r_D}\frac{\partial s_D}{\partial r_D} + K_D\frac{\partial^2 s_D}{\partial {z^2}_D} = \frac{\partial s_D}{\partial t_D} \tag{1.10}$$

Neuman regarded the water table as a moving boundary like that of Boulton (1954a) and Dagan (1967), he later linearized it and viewed the anisotropic aquifer as a three-dimensional symmetrical axis. Neumann (1974) then accounted for the penetration partially. Just like Dagan (1967), Neuman was able to reconstruct all three parts of the detected unconfined time-drawdown curve to produce estimates of parameters (along with the ability to approximate K_z) fairly similar to the models of delay yield by the use of confined storage in the governing equation (1.10).

In comparison with the models of delay index, Neuman's solution achieved similar data adjustments. Neuman (1975, 1979) interrogated the physical nature of the delay index of Boulton. He carried out a regression between the solutions Boulton (1954b) and Neuman (1972), ultimately resulting in a correlation.

$$\alpha = \frac{K_z}{S_y b}\left[3.063 - 0.567 log\left(\frac{K_D r^2}{b^2}\right)\right] \tag{1.11}$$

Expressing α significantly reduces linearly with log r and it is thus not an aquifer constant. If the logarithmic phrase in (1.11) is ignored, the relation $\alpha = 3K_z/S_y b$ implemented by Streltsova (1972a) is recovered approximately. After comprehensive analysis of various strategies for determining specific yields, Neuman (1987) deduced that the reaction of the water table to pumping is much quicker than drainage in the unsaturated area just above it. Malama (2011) has lately implemented a new linearization of roughly including the impacts of overlooked second-order terms which ultimately leads to the boundary condition of an alternative water table of:

$$S_y \frac{\partial s}{\partial t} = -K_z\left(\frac{\partial s}{\partial z} + \beta \frac{\partial^2 s}{\partial z^2}\right) \qquad z = h_0 \tag{1.12}$$

Where β represents a coefficient of linearization [L]. The variable β offers additional alteration of the physical shape of the intermediate part of the time- drawdown curve, leading to enhanced approximations of S_y.

1.7 Research objectives

This report identifies and presents the outcomes of a geohydrological study on both deterministic and stochastic groundwater analysis in the unconfined aquifer model. This study is intended to address the following questions. Firstly, what are the ethical implications of deterministic and geo-statistical methods to flow and transport modelling in real, unconfined regional aquifers? And secondly, how will vastly differing aquifer parameters influence the numerical simulations and what implications does it have in real world groundwater-related problems. We apply the two approaches (Deterministic and Stochastic models) in an attempt to answer these questions. The aims and objectives are as follows:

- To distinguish between the deterministic and stochastic model, thus say which is realistically fit to model the flow of groundwater in unconfined aquifer system
- Understanding the characteristics of the hydrogeological system and the relationship with groundwater
- To examine the main aspects of the groundwater related problems and how they could be resolved through groundwater modelling
- To utilize the models as water management and decision planning tools

1.8 Research framework

To achieve the objectives of this research, the following research framework structure was followed.

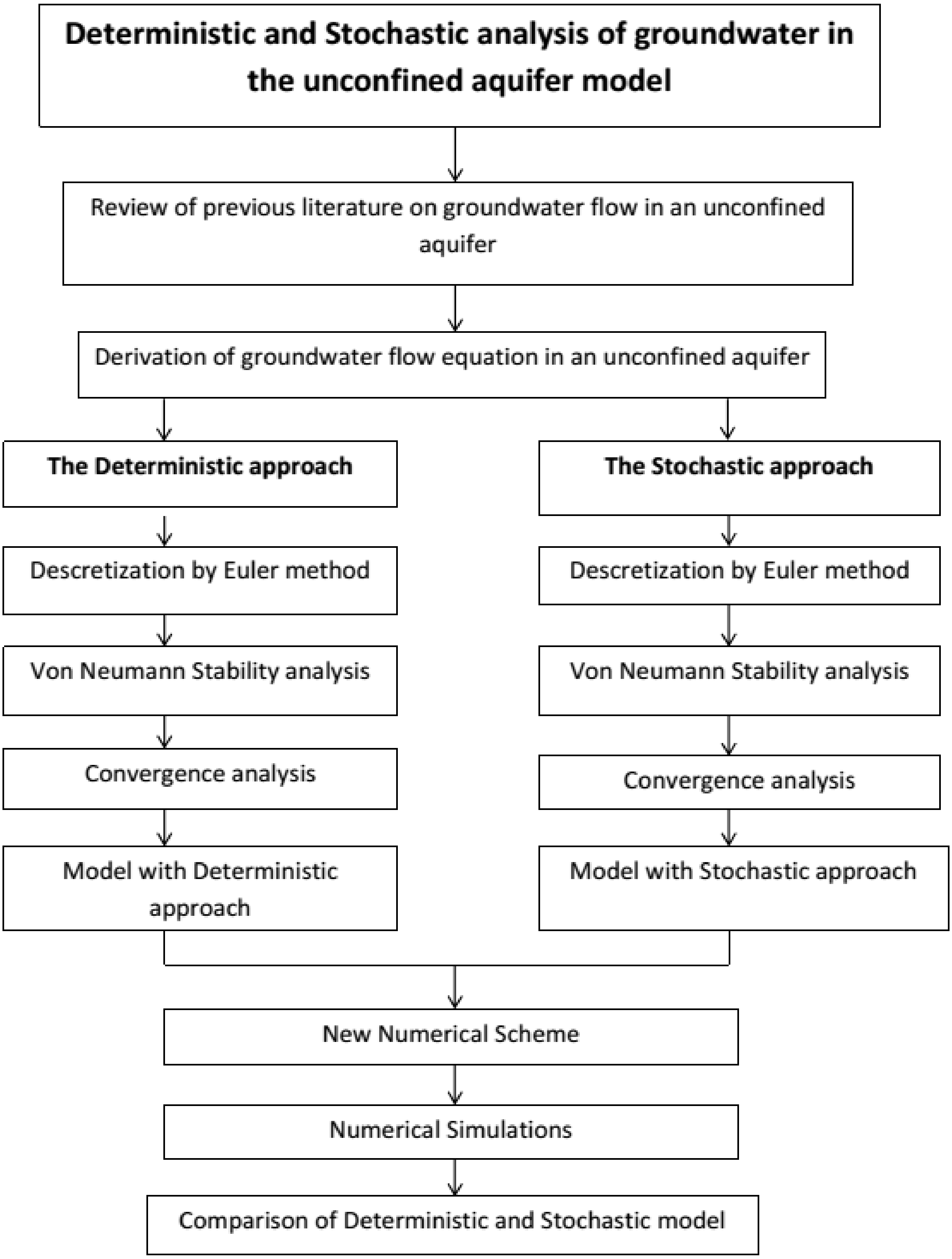

Figure 3: Theoretical framework structure followed through the research

CHAPTER TWO: LITERATURE REVIEW ON DETERMINISTIC AND STOCHASTIC MODELLING

Groundwater model constraints are generally uncertain, random and portray some kind of heterogeneity. Luckily, a vast number of model output measurements such as concentrations and heads are generally available, which accounts for inverse mathematical model formulation. Nevertheless, groundwater inversion falls short in that it has quite a number of challenges. These include Instability, non-uniqueness and many others. (Zimmerman et al., 1998; de Marsily et al., 1999; McLaughlin and Townley, 1996; Carrera, 1999; Carrera, 1987; Yeh, 1986).

Amongst many others, spatial heterogeneity is probably the hardest problem to deal with. This research is based on characterizing transmissivity (T) spatial variability. With regards to conceptual prior information as well as spatial heterogeneity, two sets of solutions can be identified: that is stochastic and deterministic. Stochastic modelling relies wholly on treating aquifer parameters as random variables. For instance, randomly treating transmissivity (T) as well as estimating its characteristics from its former measurements of T. Not only does this principle apply to transmissivity but to other aquifer parameters as well including concentrations and heads.

The dilemma was originally constructed as figuring the 'best area' in the perception of low variance or the anticipated set of measurements wired from the field (Clifton and Neuman., 1982; Kitanidis and Vomvoris., 1983; Rubinand Dagan., 1987b). Too optimistic were the estimated uncertainties derived from these solutions (Carrera and Glorioso., 1991). Perhaps this inspired the creation of implicit simulation techniques (Gómez-Hernández et al., 1997). However, these techniques presume the T from the field to be stationary. This means that these techniques are not taking into account the geological processes because they all presume that before measurements can be taken, no information is known about heterogeneity patterns.

Even though a great deal of work had been conducted on the geostatistics of geology, (e.g., Winter and Tartakovsky., 2002; Winter et al., 2003; Riva et al., 2006), most geostatistical reversal entries are predicated on this presumption of stationary status. On the other side, the deterministic approach relies wholly on the presumption that all these variability patterns of the geohydrological information are known with certainty. The process of characterising the field to account for parameters is referred to as parametrization.

By far the most commonly used technique of parametrization has to be zoning, which involves dividing the domain of the model into a number of areas. These areas are generally homogeneous with a single efficient variable value (e.g. Carrera and Neuman., 1986; Barlebo et al., 2004). Moreover, contrary to stochastic techniques, the zoning patterns in this instance are usually derived from the geohydrological data available and are specifically resolved in term of the deterministic approach. It becomes much simple and advantageous to work on zoning processes due to their flexibility to account for any geohydrological maps.

The classification of zones, however, is a quantifiable and hard-to-system project. In reality, an unacceptable classification of zones is passed on to model mechanism errors and therefore is a significant cause of failure in real projects (Sun et al., 1998). However, some measures have been taken to minimise the impact of physics errors in zones (e.g. Gaganis and Smith., 2006; Roggero and Hu., 1998). Moreover, no well-demarcated strategy was widely understood. The deterministic approach is disadvantageous in that it turns to neglect the impacts of small scale heterogeneities during modelling.

Hence, the geostatistical measurement mechanism embodies the conceptual fine detail better than that which can be captured with a limited number of zones. Nonetheless, zoning is and always has been the preferred method in the geohydrological field, especially in local or basin-scale underground water models (e.g., Senger and Fogg., 1987; Guymon and Yen., 1990; Castro et al., 1998; Walvoord et al., 1999; Shavit and Furman., 2001; Best and Lowry., 2014; Ala-Aho et al., 2015; Nocchi and Salleolini., 2013, etc.).

The stochastic approach was immediately enforced in instances where geohydrological data is not sufficiently powerful to enable for the predefinition of such spatial heterogeneity trends. As a result, field projects are limited to comparatively minor problems, in which the geohydrology and geology is not all that binding and the pressures and reactions are well characterised.

In terms of stochastic studies, not so much of major and complicated problems have been investigated. In previous research that has been done, Rubin and Dagan (1987a, b) and Clifton and Neuman (1982) utilised the stochastic reversal approach to model the steady-state Avra Valley aquifers. In addition to the previously conducted studies on the stochastic approach, Rubin et al (1990) further proved the validity of the Rio Mayor Aquifer as well as the Israeli Coastal Aquifer stochastical approach studies respectively. These instances have demonstrated to be effective during the initial stages of the technique. They did not reveal its credibility, however, that is generally the case in real-global scale implementations since not so much information is provided to measure the model entirely independently.

In reality, there is still a very significant complete absence of implementations of stochastic conjectures and global scale strategies in the real world till this day (Neuman., 2004; Dagan., 2002). Latest exclusions include Jardani et al.'s works. (Dausman et al., 2012). This absence is far more prevalent in the case of reversal geostatistical flow and transport information. We say the biggest problem lies in disregarding hydrogeological and geological specific information, which happens to have many details on a global scale rather than a small scale. In other words, geological complexity trends (and hydraulic heterogeneity) are widely known at global level. It would be bad habit to ignore them.

Therefore, experts usually find that somehow readily accessible stochastic solutions do not integrate geological accurate information and generally prefer deterministic strategies when faced with a global model. Instead, local geological information less than a kilometer is generally far less precise and heterogeneity patterns cannot really be suggested a priority. Parsimony validates stationarity as the previous model in these cases, which demonstrate the wide use and popularity of small stochastic models. A lot of time and effort was put into overcoming this restriction of stochastic strategies.

The most profitable efforts may be based entirely on heterogeneity categorization in terms of hydrogeological faces. Transitional models based primarily on Markov chains (TPMC) examine mathematical variability and produce equally probable discoveries of geological units or facies. TPMC techniques are a strong geostatistical strategy for predicting geological facies allocation using generalised indicator parameters (e.g., Ritzi., 2000 Carle and Fogg., 1996, 1997; Fogg et al., 1998; Elfeki and Dekking., 2001)

These solutions have already been simplified making use of geostatistics and connectivity notions from various points (Renard and Allard., 2013) In practice, these strategies entail the generation of both a vast number of lithofacies or otherwise hydraulic conductivity areas as well as the rejection from those who do not respect the heads discovered (e.g., Sakaki et al., 2009; Zhou et al., 2012; Alcolea and Renard., 2010; Berg and Illman., 2011; Khodabakhshi and Jafarpour., 2013).

The other strategies to replicate real trends of heterogeneity are predicated mostly on geophysical raw data to accommodate for the shortages of hydrological readings in situ as well as to improve the performance of the depiction of geostatistics (e.g., Rubin et al., 1992; Copty et al., 1993; Hyndman et al., 1994; Hubbard et al., 1997; Ezzedine et al., 1999; Hubbard and Rubin., 2000) Though all these strategies look very appealing, their implementation to realistic global structures is already in stages of development.

In view of the latter constraints, the initial critical and interesting question one could ask is whether the stochastic strategy is appropriate for modelling real global aquifers or whether the reverse problem is properly dealt with it in a deterministic structure. The original source of T data is a unique crucial question provided that one uses the stochastic reverse technique. Most of these are typically accessed mostly from long periods of pump tests which tend to be costly. Extra T raw data could also be extracted from all of precise capacities (pumping rate, Q, divided by drawdown, s).

Specific capacity (SC) is referred to as the variable that is most commonly supplied by step-down exam contractors to classify a well's performance. Therefore, SC raw data are sometimes more easily obtainable as compared to T raw data. Ahmed and Marsily (1987), as well as Clifton and Neuman (1982), emphasised that raw data obtained from either pumping tests or specific capacity could yield better estimates of the T field data.

Meier et al., (1999) on the one side has demonstrated that perhaps both measurements typically depict varying scales. Specific capacity estimations rely heavily on transmissivities in the nearest area of the well, although pumping test ideologies are sensitive to the duration of the test and tend towards effective transmissivities over time. Thus, the upgrading of T raw data from well-scale to aquifer scale while taking into consideration the geological context is a major issue faced by hydrogeologists. This leads us to wonder whether these two kinds of T calculations are suitable for global aquifers. This study is aimed at addressing the above questions. What are the relative merits of deterministic and geostatistical approaches for the modelling of flow and transport in real regional unconfined aquifers?

The Water Resources Research released an article through which by analysing the appropriate papers on groundwater modelling in a stochastic structure. Dagan (1986) indicated that this new research, defined by an extremely rapid increase in the number of publications, and it is on the stage and is maturing. By making use of the integral equation formulation, Cheng and Lafe (1991) portrayed a solution to the issue of stochastic boundary value in groundwater flow.

The type of aquifer that was regarded had a hydraulic conductivity for the deterministic model. This aquifer, however, seems to be prone to some kind of random boundary condition. Geostatistical integral equations for the covariance, mean, flux and head are developed using a distribution source. For mathematical solutions, a constant boundary element method is introduced. Two uniform instances are investigated and particularly compared with the precise solution. There's then a two-dimensional problem which becomes more complex. New stochastic numerical schemes are continuously developed to cater for even more complex problems.

2.1 Approaches for spatial variability

2.1.1 The deterministic approach

For the past years, geohydrologists have depended on deterministic strategies in several extremely high heterogeneous aquifers to anticipate flow and solute transport particularly in groundwater. As already stipulated in the above chapter, the deterministic system's variables are specified in the answer domain at all key points in a mathematical model. The deterministic strategy may be split evenly into a homogeneous and heterogeneous equivalent strategy. The equivalent homogeneous strategy presumes that yet another heterogeneous aquifer can be allowed to behave as a homogeneous equivalent in space. However, the hydraulic properties are kept constant.

These constant variables are referred to as effective variables and are commonly acquired by vast hydraulic tests. These values can also be obtained from getting an average value from all these small tests. For instance, getting an average from the geometric, harmonic and arithmetic means of a pumping test's transmissivity values. These effective values that are certainly known will be used as input parameters. These input parameters can be used to run mathematical models and it is these models that will be used to anticipate possible contamination if any or simply, the general flow of water. On the other hand, the heterogeneous strategy uses all available field data to determine the heterogeneity of the aquifer. The latter approach is implemented in order to identify how groundwater behaves as well as how contaminants could possibly be transported from one place to the other.

Whether the aquifer is regarded as homogeneous or heterogeneous, deterministic strategies have several disadvantages. First, there really is no scientifically valid way of acquiring effective variables of the equivalent homogeneous aquifer by making use of raw data from hydraulic tests on a massive scale. For instance, it is necessary to establish just how many monitoring boreholes are needed to correctly use Theis' solution to measure effective transmissivity. This implies that, the previous question about the accuracy between both the field data scales and the Representative Elementary Volume (REV) of the model is never addressed. Small scale hydraulic tests can often give wrong interpretations. For instance, transmissivity or slug test measurements using of core samples are expected to vary with hydraulic variable measurements in different parts of the aquifer. Practical relevant questions would be: how do we average the data to achieve the hydraulic variables for the homogenised equivalent aquifer?

And if such an efficient hydraulic conductivity can be represented, how can we link the observations to the presumed results. The heterogeneous strategy also falls short in that there is limited data from small scale tests for predictions to be made especially about the transportation of contaminants. How can aquifer property values be assigned from areas where no readings have been made? What is the extent of the uncertainty in our forecasts if there is only a small number of data? A deterministic strategy is essential in answering these questions, and a stochastic strategy is by far the most realistic. (Camel and Hanna.; 1995)

2.1.2 The stochastic approach

Though ideas predicated on stochastic strategies to solve spatial variability issues have also been established in groundwater in the past few years. Several recent field studies in both saturated zones (Freyberg., 1986; Sudicky., 1986; Garabedian et al., 1991) and unsaturated zones (Yeh et al., 1986; Greenholtz et al., 1988; McCord et al., 1991) have indeed noted that the stochastic strategy is instituted in the following sections through the first discussion of the concept of statistics to depict heterogeneity. Lately, researchers are developing stochastic mathematical equations that will account for groundwater related problems. Lastly, more recent studies are developing theories of depicting the transport of contaminants in groundwater problems in global scale aquifers.

2.2 Statistical representation of heterogeneity

On different assessment scales, aquifers are demonstrably heterogeneous. The depiction of heterogeneity on a scale of our own genuine importance typically involves hydrological relevant information on every juncture in the aquifer. Determining a very comprehensive distribution of hydraulic properties in aquifers of tens of kilometers of size effectively requires various measurements, longer time and great costs and is frequently regarded impractical and unfeasible. The real solution is to get a small quantity of data to approximate parameter heterogeneity in a statistical context.

In other words, the variability of a property is defined by its approximated probability dispersion of samples. Hoeksema and Kitanidis (1985) proposed the log-normal distribution of the storage coefficient. The distributions of hydraulic conductivity are normally log-normal (Warren et al., 1961; Bakr., 1976; Bulness., 1946; Law., 1944; Freeze., 1975; and Sudicky., 1986; Jensen et al., 1987).

Freeze (1975) regarded hydraulic conductivity as a randomly chosen variable based on this statistical approach and examined the uncertainty of groundwater flow modelling. The latest evaluates of hydraulic conductivity data by (Bakr., 1976; Byers and Stephens., 1983; and Hoeksema and Kitanidis., 1985) depicted that the measurements of hydraulic conductivity vary in space. However, this variation in space is strongly correlated rather than completely random. This correlation in space entails that these parameters are not independent of the stochastic nature and thus should be regarded as stochastic parameters and not randomly chosen variables.

Illinois (Bakr, 1976) describes a practical example on the hydraulic conductivity raw data tested across a borehole in sandstone and used it to describe the stochastic spatial variability of hydrological variables, see figure 4. At a particular point within the borehole, the hydraulic conductivity value can be recognized as one of several other possible geological formations that had deposited at that particular point. Therefore, at that particular point the hydraulic conductivity becomes a random variable $K(x_0, \omega)$. The ω indicates that many possible K values are x_0. Likewise, hydraulic conductivity values are random variables at other locations along the boron hole. El-Kadi (1995)

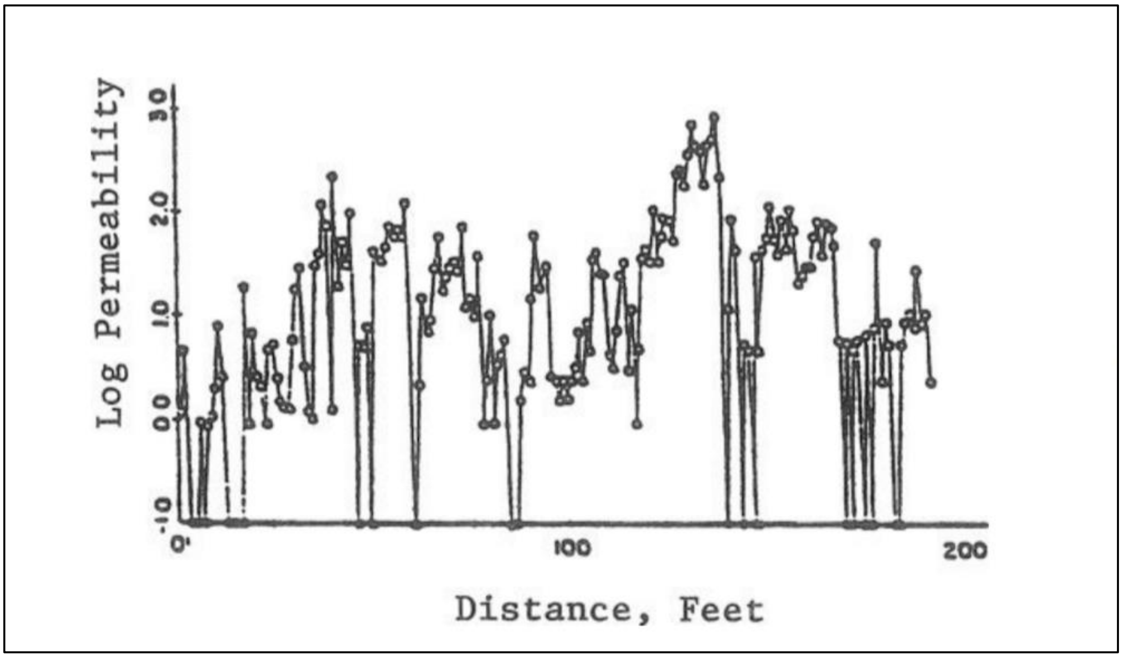

Figure 4: Hydraulic conductivity values of Mt Simon sandstone depicting variability of the Hydraulic parameter (EL-Kadi, 1995)

Consequently, all of the values of hydraulic conductivity of the whole borehole depth can then be regarded as a compilation of random variables in space. In other words, if the measured value of hydraulic conductivity is obtained at the point at $x_1, x_2, x_3 \ldots.. x_n$, it can only make sense that $K(x_1, \omega)$ represents its random variable, $K(x_2, \omega)$ represents an additional random variable. This pattern goes on and on to $K(x_n, \omega)$. Thus, each will have a dispersion of probabilities but this dispersion of probabilities can also be linked. The likelihood of having a specific pattern of values of hydraulic conductivity along the whole borehole $K(x, \omega_1)$, does not only confide for the probability dispersion of the hydraulic conductivity at a particular point, but also at others.

This means that a real value of hydraulic conductivity is a predictable succession of $K(x, \omega_1)$ out of all predictable successions, $K(x, \omega)$.The likelihood of discovering a sequence in the terminology of stochastic processes would then be referred to as the common probability distribution. These probable successions are referred to as an ensemble.

A joint distribution of such randomly chosen variables should be generally known to identify the likelihood of occurrence of a specific succession of random variables. The joint distribution is entirely described only if the variables that are correlated with all the probable sequences of $K(x, \omega)$ are known within a borehole. Evidently, this joint distribution is realistic situations because the values of hydraulic conductivity that were measured along the entire borehole were then geostatistical data set, analysed stochastically and accounting for variability that occurs naturally which is often neglected by humankind. Thus, non-complex terms must be used to describe these theories. The terms are referred to as stationary and ergodicity and these terms are further described.

The term stationarity refers to all the statistical properties of a stochastic process such as variance, mean or joint distribution. These properties are always kept constant or stationary in space. Ergodicity simply implies that by recognizing the variability in just a single geological formation, one can possibly obtain the statistical properties of the stochastic process for all the geological formations. It is evident enough or rather safe to say that one has no meaningful choice than to assume that ergodicity has a potential and realistic explanation for the stochastic strategy.

Because stationarity is one of the most essential terms of the stochastic process, it can also be expressed by means of geostatistical equations referred to as moments. For instance, a Mean represents a first "moment" while a Variance represents a second "moment". These are generally used to distinguish if the stationarity is of first or second order. Below is the first mean $K(x)$ expressed as:

$$\mu = E[K] = \int_0^{\infty} Kf(K)dK \tag{2.1}$$

Here, $E[K]$ represents the expected value, that is; the mean over the whole ensemble. The joint density distribution of K is expressed as $f(K)$. The covariance is therefore expressed as:

$$c(\xi) = cov[K(x+\xi), K(x)] = E[(K(x+\xi) - \mu)(K(x) - \mu)] \tag{2.2}$$

Here, the mean is kept constant while the covariance is dependent on the mean. This is referred to as Second-order stationarity. In order to calculate the covariance, the following assumption had to be made:

This assumption enables everyone else to classify the stochastic mechanism just by using its mean and covariance function. If the distance of separation is assigned to be zero, the covariance parameter is the variance. A correlation coefficient parameter is generally described as the relationship between the covariance and its variance.

$$\rho(\xi) = \frac{c(\xi)}{\sigma^2} \tag{2.3}$$

The correlation coefficient’s parameter is the consistency of a property's value in space. In particular, the correlation coefficient’s parameter of the hydraulic conductivity is inversely proportional to the distance. When the hydraulic conductivity vastly decreases, the distance increases. The correlation coefficient's behaviour can be simulated by means of a different number of models. The correlation decrease can be represented by many different models of autocorrelation. An exponential downturn model is frequently used (Bakr et al., 1978; Yeh et al., 1985 a,b,c Gelhar and Axness., 1983):

$$\rho(\xi) - exp\left\{-\left[\left(\frac{\xi_1}{\lambda_1}\right)^2 + \left(\frac{\xi_2}{\lambda_2}\right)^2 + \left(\frac{\xi_3}{\lambda_3}\right)^2\right]\right\} \tag{2.4}$$

Where ρ represents the correlation co-efficient value. The separation vector is denoted by the symbol, ξ and the correlation scales in the directions $x, y,$ and z respectively are λ_1,λ_2 and λ_3. The integral scale stands as a denominator and thus cannot be a non-positive or a zero value. (Lumley and Panofsky.,1964);
(El-Kadi., 1995)

2.3 Numerical simulation

Numerical simulation is a viable device with analytic capacity used to solve groundwater management sustainability problems (Ghassemi et al., 1997; Narayan et al., 2007; Ayvaz et al., 2008; Rejani et al., 1997; Ayvaz et al., 2008, 2009; 2014; Lu et al., 2013). The computer simulation outcomes of established or outlined groundwater management mechanisms can help locate the viable percentage of groundwater and an acceptable long term groundwater management strategy (Paniconi et al., 2001; Zhou et al., 2001; Barazzuoli et al., 2003).

Stochastic computation is a simulation where some parameter or mechanism is restricted by stochastic factors and processes and predicted using pseudo-random data based on Monte Carlo strategies, and it also reproduced runs of the same kind of boundary conditions are expected to generate different results within a specific band of trust. Deterministic computation is a visualization wherein the parameter is governed by deterministic methodologies, and it also reproduced runs from the very same limits also always yield results that are similar.

The simulation of anything most first enables the creation of a new model; this model encompasses the key elements, habits and processes of the physical or conceptual system or mechanism chosen. The growth model is the system itself, while the visualization symbolizes the system's long-term apparatus. Below is a flow diagram depicting some of the disciplines that are essential for basic simulation.

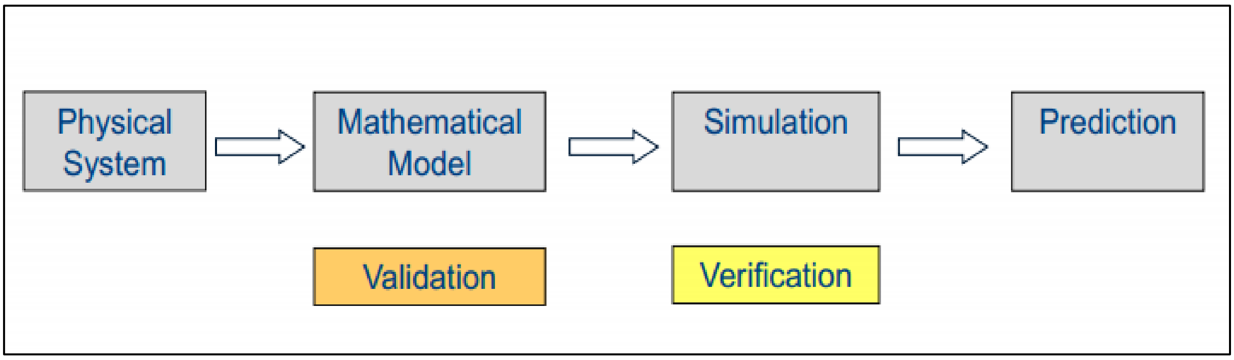

Figure 5: The main elements of simulation (Chandio *et al,* 2012)

Validation : Make absolutely sure that the right math model is dealt with.

Verification: Help to ensure the mathematical model is appropriately solved.

CHAPTER THREE: THE USE OF NUMERICAL MODELS TO SIMULATE GROUNDWATER FLOW AND TRANSPORT

3.1 Numerical models

The term model has many other understandings and is sometimes misused that perhaps the definition of the word can often be extremely hard to distinguish (Konikow and Bredehoeft.,1992). Thus, most often its definition is broken to a simple, and much more realistic one. A model is most simply a characterization of a real system or framework. A concept model is a simple prediction of the operation of a system or mechanism. This implication can be explained often as a mathematical model in quantitative terms. Mathematical models are derivations which encompass mechanisms as mathematical models, physical characteristics as constants or coefficients in equations and state or potential measurements in the system as parameters.

The majority of groundwater models used today are mathematical deterministic models. The deterministic models rely wholly on mass conservation, energy and momentum. These type of models characterises the relationship between input and output. The basic assumption here is that the reaction of the system to any other set of stresses can be clearly defined, even if completely new stresses fall outside the range of predominantly observed stresses, the system's reaction to any new set of stresses can be obtained.

In particular, deterministic groundwater models involve partial differential equations to be resolved. Exact solutions can indeed be analysed, but analytical models involve extremely variables and boundaries. Most of these deterministic models regard the properties of the porous media to be represented as combined parameters. This only means that the heterogeneous parameters are disregarded in the entire model. Variability or randomness in aquifer parameters is descriptive of the geological nature and is already known to have an essential role in impacting groundwater behaviour and how contaminants can be tracked from flow and transport processes.

It is therefore always advantageous to use dispersed parameter models which enable more practical data sets of system properties to be represented. Discrete mathematics provides estimated solutions to the equation by discretizing the partial derivative equation in space and time. Once the discretized equation is derived from the partial derivative equation, the variable internal characteristics, stresses and limits of the system are estimated. Therefore a distribution parameter needs to be introduced to the deterministic model to account for the heterogeneity that was disregarded from the aggregated deterministic models. In that way, the stochastic models will thus be more realistic.

3.2 Flow and transport processes

The groundwater flow mechanism is usually affirmed to be governed by the relationships conveyed in Darcy's law and mass conservation. But again, Darcy's law seems to have no limits on its scope of application and these limitations should be assessed in every implementation. The real intent of a model that emulates the flow transportation of a solute in groundwater is to be able to measure the cognitive function of the dissolved species at a certain time and place in an aquifer. Alterations in chemical abundances are mainly due to four different processes in a dynamic groundwater scheme:

1) Advective transport, here, the already dissolved chemicals flow together with groundwater.
2) Hydrodynamic dispersion, in this process, a minor-scale variation of the flow velocity as well as ionic and molecular diffusion creates a path of molecules that are dissolved, through which the ions diverge and start to spread out from the water flow direction.
3) A fluid source, water of a single composition is introduced into water of different compositions. The water eventually mixes.
4) Reactions, a specific amount of chemical species that is dissolved could be introduced or removed from groundwater resulting from different reactions that occur in groundwater. These reactions could be physical, biological or chemical.

The hydrogeological environment is a complex, heterogeneous subsurface setting that is three-dimensional and very diverse. This heterogeneity drastically alters the flow and transport of groundwater, so this essence could only be defined by careful hydrogeological exercise when in the field. Irrespective of just how much information is obtained in the field, the boundary conditions and some properties of the groundwater system stay uncertain. Stochastic solutions have led to many major improvements in portraying the variability of the subsurface and addressing uncertainty (Gelhar.,1993).

3.3 Groundwater flow equation

The rate of such water flow through a permeable medium relates once again to the characteristics of the water, the characteristics of the permeable medium and the slope of the hydraulic head, as defined by the law of Darcy. It can be denoted as:

$$q_i = -K_{ij} \frac{\partial h}{\partial x_j} \qquad (3.1)$$

In the above equation, q_i represents the specific discharge, while the hydraulic conductivity is represented by LT^{-1}, K_{ij}. The hydraulic conductivity is of a porous medium referred to as a second order tensor, $LT^{-1}h$; and h represents the hydraulic head, L. A particular type of the equation discussing the transient flow of a very conductive liquid and in a completely non- homogeneous anisotropic aquifer can be extracted through the combination of the law of Darcy and a continuity equation. In Cartesian tension equations, a particular groundwater flow equation can be written as:

$$\frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial h}{\partial x_i}\right) = S_s \frac{\partial h}{\partial t} + W^* \qquad (3.2)$$

Where the transmissivity is represented by T_{ij} and T_{ij}= K_{ij}, b is known to be the aquifer's saturated thickness, S represents the storage coefficient and $W^* = W^* * b$ is the volume flux per unit area, LT^{-1}.

When equation (3.2) has adhered to such an unconfined (water-table) aquifer scheme, then it should be thought that the flow is horizontal or lines are vertical, that the slope of the horizontal hydraulic is equivalent to the water table incline and that the storage coefficient is equivalent to the specific yield S_y (Anderson and Woessner.,1992). Bear in mind that even the saturated thickness in an unconfined system changes with the water table elevation (or head). It becomes obvious that the transmissivity also changes in space and over a period of time. However, the properties of the fluid such as viscosity and density can be significantly different in both space and time. This can happen as soon as the temperature of the fluid or the concentration of dissolved solids alters greatly. However, the relation between the water levels, fluid velocity, and fluid pressure becomes easier to understand, provided that the properties of the fluid are transient or heterogeneous. In these instances, the flow equation is then resolved based on fluid properties such permeability, density of the fluid, fluid pressure, etc. (Konikow and Grove.,1977). The research framework followed in this study is depicted in figure 6.

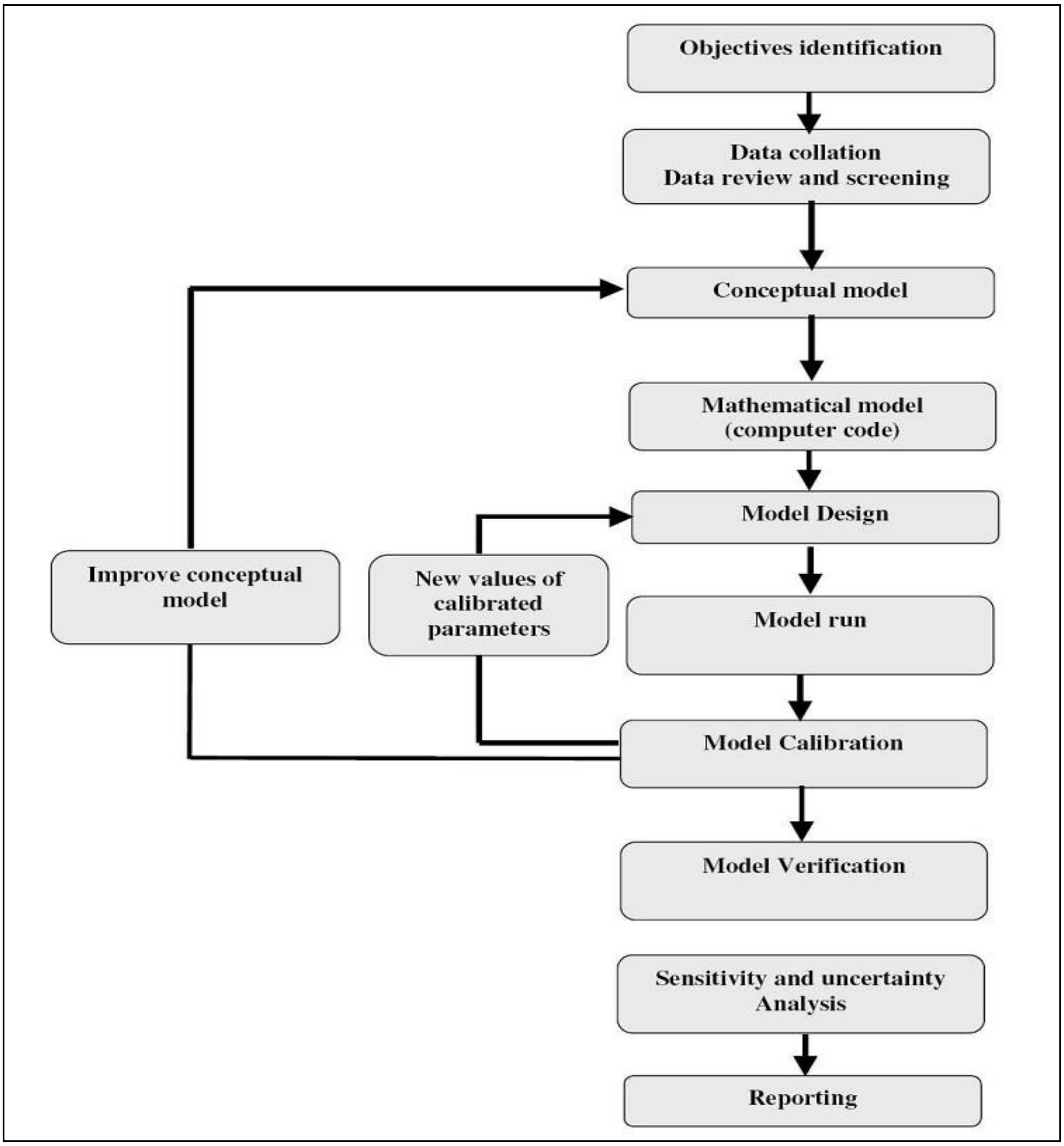

Figure 6: Research framework followed through this research

CHAPTER FOUR: ANALYSIS OF THE DETERMINISTIC MODEL

4.1 Introduction to discretization

Discretization in simple terms is deriving a difference equation. It is an approximation to the differential equation, which involves only differences in function values, i.e. no derivatives in the equation. The difference equation's solution is expressed as a discrete function and not a continuous function.

By using several varying viewpoints, The Euler method can be derived. Firstly, the derivative in the differential equation has to be substituted by an approximation.

From basic mathematics, we can define the derivative of any given function at the points $y(t)$ and $t = a$ as:

$$y'(a) = \lim_{h\to 0}\frac{y(a+h) - y(a)}{h} \tag{4.1}$$

From a graphical perspective, the slope of the secant that merges $(a;\, y(a))$ and $(a + h; y(a+h))$ is used. It is very essential to note that the slope of the secant becomes closer to that of the tangent line at a when $a + h$ approaches a which is denoted by $y'(a)$. The difference quotient then becomes:

$$y'(t_0) \approx \frac{y(t_1) - y(t_0)}{\Delta t} \tag{4.2}$$

The above equation denotes an estimation to $y'(t_0)$. From this equation, we have to generate a difference equation. By so doing, Y_i then represents our estimation to $y(t_i)$. It becomes obvious that $Y_0 = y_0$. The difference equation produced at t_0, is then used to produce the Euler method at t_1. The differential equation $y_0(t) = f(t; y(t))$, is used together with the estimation $y'(t_0)$ to obtain:

$$\frac{Y_1 - Y_0}{\Delta t} = f(t_{0,}Y_0) \tag{4.3}$$

From the above equation, the starting point is denoted as Y_0 resulting from the starting condition. Therefore if the initial conditions are set, then one can calculate fore $y(t_1)$. This results in:

$$Y_1 = Y_0 + \Delta t f(t_{0,}Y_0) \tag{4.4}$$

As soon as the difference equation for Y_1 is calculated, a similar process can be performed again to produce the difference equation for Y_2. The general notation then becomes:

$$Y_{i+1} = Y_i + \Delta t f\left(t_{i,} Y_i\right) \tag{4.5}$$

This is referred to as the Forward Euler method.

Using the forward Euler method as a guide to solve derivative equations, we can employ that:

$$\frac{\partial C}{\partial t}(x_i t_n) \tag{4.6}$$

$$\frac{\partial C}{\partial t}(x_i t_n) = \frac{C(x_i, t_{n+1}) - C(x_i, t_n)}{\Delta t} \tag{4.7}$$

$$= \frac{C_i{}^{n+1} - C_i{}^{n}}{\Delta t} \tag{4.8}$$

Similarly, using the forward Euler method to solve second derivative equations, we can employ that:

$$\frac{\partial C}{\partial t}(x_i, t_n) = \frac{C(x_i, t_{n+1}) - C(x_i, t_n)}{\Delta t} \tag{4.9}$$

$$\frac{\partial^2 C}{\partial x^2}(x_i, t_n) = \frac{C(x_{i+1}, t_{n+1}) - 2C(x_i, t_{n+1}) + C(x_{i-1}, t_{n+1})}{(\Delta x)^2} \tag{4.10}$$

$$= \frac{C_{i+1}{}^{n+1} - 2C_i{}^{n+1} + C_{i-1}{}^{n+1}}{(\Delta x)^2} \tag{4.11}$$

Using the forward Euler to discretize a differential equation, we can employ that:

$$\int_0^t \frac{\partial s^*}{\partial \tau} e^{-\alpha(t-\tau)} d\tau = \int_0^{t_n} \frac{\partial s^*}{\partial \tau} \exp(-\alpha(t_n - \tau)) d_\tau \tag{4.12}$$

$$= \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} \frac{f^{j+1} - f^j}{\Delta t} exp[-\alpha(t_n - \tau)] d_\tau \tag{4.13}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^j}{\Delta t} \int_{t_j}^{t_{j+1}} exp[-\alpha(t_n - \tau)] d_\tau \tag{4.14}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^j}{\Delta t} \int_{t_n - t_{j+1}}^{t_n - t_j} exp[-\alpha y] d_y \tag{4.15}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^{j}}{\Delta t} \left(-\frac{1}{\alpha}\right) \int_{t_n - t_{j+1}}^{t_n - t_j} -\alpha exp[-\alpha y] d_y \tag{4.16}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^{j}}{\Delta t} \left[-\frac{1}{\alpha} exp(-\alpha y)\right] \tag{4.17}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^{j}}{\Delta t} \left(-\frac{1}{\alpha}\right) - exp\left(t_n - t_j\right) - exp\left(t_n - t_{j+1}\right) \tag{4.18}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^{j}}{\Delta t} \left(-\frac{1}{\alpha} exp\left(t_n - t_j\right) + exp\left(t_n + t_{j+1}\right)\right) \tag{4.19}$$

$$= \sum_{j=0}^{n} \frac{f^{j+1} - f^{j}}{\Delta t} \left\{\left[\frac{exp[\Delta t(n-j)] - exp[\Delta t(n-j-1)]}{\alpha}\right]\right\} \tag{4.20}$$

Applying the Forward Euler method to discretize the unconfined aquifer equation, we can employ that:

$$\frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r} = \frac{S}{T}\frac{\partial s}{\partial t} + \left\{\alpha S_y \int_0^t \frac{\partial s^*}{\partial \tau} e^{-\alpha(t-\tau)} d\tau\right\} \tag{4.21}$$

$$\frac{S\left(r_{i+1,}t_{n+1}\right) - 2S\left(r_{i,}t_{n+1}\right) + S\left(r_{i-1,}t_{n+1}\right)}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S\left(r_{i+1,}t_{n+1}\right) - S\left(r_{i,}t_{n+1}\right)}{\Delta r}\right)$$
$$= \frac{S}{T}\left(\frac{S\left(r_{i,}t_{n+1}\right) - S\left(r_{i,}t_{n}\right)}{\Delta t}\right) + \alpha S_y \sum_{j=0}^{n} \frac{S\left(r_{i,}t_{j+1}\right) - S\left(r_{i,}t_j\right)}{\Delta t} \tag{4.22}$$

$$We\ let\ S(r_i, t_n) = S_i^{\,n}$$

$$\frac{S_{i+1}{}^{n+1} - 2S_i^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i^{\,n+1}}{\Delta r}\right)$$
$$= \frac{S}{T}\left(\frac{S_i^{\,n+1} - S_i^{\,n}}{\Delta t}\right)$$
$$+ \alpha S_y \sum_{j=0}^{n} \frac{S_i^{\,j+1} - S_i^{\,j}}{\Delta t}\left\{\left[\frac{exp\left[\Delta t(n-j) - exp[\Delta t(n-j-1)]\right]}{\alpha}\right]\right\} \tag{4.23}$$

$$\frac{S_{i+1}{}^{n+1} - 2S_i^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i^{\,n+1}}{\Delta r}\right)$$
$$= \frac{S}{T}\left(\frac{S_i^{\,n+1} - S_i^{\,n}}{\Delta t}\right) + \alpha S_y \sum_{j=0}^{n} \frac{S_i^{\,j+1} - S_i^{\,j}}{\Delta t} \delta_{j,n}{}^{\infty}$$

$$\frac{S_{i+1}{}^{n+1} - 2S_i^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i^{\,n+1}}{\Delta r}\right) \tag{4.24}$$
$$= \frac{S}{T}\left(\frac{S_i^{\,n+1} - S_i^{\,n}}{\Delta t}\right) + \alpha S_y \sum_{j=0}^{n-1} \frac{S_i^{\,j+1} - S_i^{\,j}}{\Delta t}$$
$$+ \sum_{j=0}^{n+1} \frac{S_i^{\,n+1} - S_i^{\,n}}{\Delta t}\ \frac{1 - e^{-\Delta t}}{\alpha} \tag{4.25}$$

This discretized equation will be used to perform many other analyses such as the stability analysis for both models. That is, Stochastic and deterministic.

4.2 Stability analysis

4.2.1 Von Neumann stability analysis

In the past decades, the Von Neumann's stability method which is also referred to as the Fourier's stability method has been and is still in operation to date. It is generally used to perform stability analysis on finite differential equations. The estimate is based on the decay of numerical errors in Fourier. This scheme was implemented at the Los Alamos Regional Lab by the British researchers Crank and Nicolson in 1947. This scheme became popular and many scientists started to utilise it.

The stability of a finite difference scheme is reached if the error at that particular point does not result in an increase in errors as the mathematical calculations continue. A rationally stable system remains constant when calculations are carried on. So if the errors decline and finally dampen, the numerical system is stable. On the contrary, if the errors increase over time, the numerical scheme becomes unstable. Thus, the Von Neumann method becomes a crucial tool to examine the stability of any linear or differential equation.

In essence, the numerical errors (round off due to final precision of computers) should not be allowed to grow unboundedly and the numerical solution itself should remain uniformly bounded. For time-dependent problems, stability guarantees that the numerical method produces a bounded solution whenever the solution of the exact differential equation is bounded. Stability, in general, can be difficult to investigate, especially when the equation under consideration is nonlinear.

In some instances, Von Neumann stabilization is appropriate and feasible for stability analysis in the perception of Lax-Richtmyer (which was utilised in the Lax equivalence theory): the finite differential model as well as the partial differential equation (PDE) are linear. The PDE is fairly constant with continuous limit conditions but only has two independent parameters. Stability of Von Neumann is essential in a much wider range of instances. It is mostly used rather than a more complicated and detailed stability analysis. This is done so that one gets a good understanding of the restrictions on the steps used in the scheme due to its relatively straight-forward.

The Von Neumann mechanism is based solely on the error breakdown into the series of Fourier. Consider the following one- dimensional heat equation to emphasise the method:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{4.26}$$

The discretization of the equation is as follows:

$$u_j{}^{n+1} = u_j{}^n + r\left(u_{j+1}{}^n - 2u_j{}^n + u_{j-1}{}^n\right) \tag{4.27}$$

Where:

$$r = \frac{\alpha \Delta t}{\Delta x^2} \tag{4.28}$$

The solution $u_j{}^n$ of the linear equation simulates the PDE analytical solution $u(x,t)$ on the national grid.

Define the round-off error $\epsilon_j{}^n$ as

$$\epsilon_j{}^n = N_j{}^n - u_j{}^n \tag{4.29}$$

The $u_j{}^n$ is the ultimate solution of the discretized equation which would be calculated in the lack of a round-off error, and $N_j{}^n$ is the alternative of the numerical solution acquired in finite accuracy arithmetic. Because the exact solution should accurately comply with the discrete equation, the error $\epsilon_j{}^n$ must also comply with the discrete equation. Here however we presumed that the $N_j{}^n$ complies with the equation. Thus:

$$\epsilon_j{}^{n+1} = \epsilon_j{}^n + r\left(\epsilon_{j+1}{}^n - 2\epsilon_j{}^n + \epsilon_{j-1}{}^n\right) \tag{4.30}$$

The above equation represents an error recurrence relationship. For linear partial differential equations with sporadic boundary condition, the spatial variability of error in a Fourier series can be broadened in the L interval,

$$\epsilon(x) = \sum_{m=1}^{M} A_m \, e^{ik_m x} \tag{4.31}$$

Here, the wavenumber $k_m = \frac{\pi m}{L}$ with $m = 1,2,3, \dots, M$ and $M = \frac{L}{\Delta x}$. The time dependency of the error is featured in the presumption that the error amplitude A_m is a time parameter. Seeing that the error tends to exponentially increase or decrease over time, it is logical to assume that the amplitude fluctuates exponentially over time, hence:

$$\epsilon(x,t) = \sum_{m=1}^{M} e^{at}\, e^{ik_m x} \tag{4.32}$$

Where a is a constant.

Because the error difference equation is linear (the conduct of every phrase in the series is the same as the series itself), the error growth of a fairly typical phrase is sufficient:

$$\epsilon_m(x,t) = e^{at} e^{ik_m x} \tag{4.33}$$

The characteristics of stability can be examined by utilising this form for the error without loss in general.

$$\varepsilon_j{}^n = \ exp[at]exp[ik_m x] \tag{4.34}$$

$$\varepsilon_j{}^{n+1} = exp[at]exp[ik_m(x+\Delta x)] \tag{4.35}$$

$$\varepsilon_{j+1}{}^{n+1} = \ exp[a(t+\Delta t)]exp[ik_m(x+\Delta x)] \tag{4.36}$$

$$\varepsilon_{j-1}{}^{n-1} = \ exp[a(t-\Delta t)]exp[ik_m(x-\Delta x)] \tag{4.37}$$

to yield (after simplification)

$$e^{a\Delta t} = 1 + r\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x} - 2\right) \tag{4.38}$$

Using the identities

$$sin\left(\frac{k_m\Delta x}{2}\right) = \frac{e^{ik_m\Delta x/2} - e^{-ik_m\Delta x/2}}{2i} \ \rightarrow \ sin^2\left(\frac{k_m\Delta x}{2}\right) = -\frac{e^{ik_m\Delta x} + e^{-ik_m\Delta x} - 2}{4} \tag{4.39}$$

Equation (4.38) may be written as

$$e^{a\Delta t} = 1 - 4r sin^2\left(\frac{k_m\Delta x}{2}\right) \tag{4.40}$$

Define the amplification factor

$$G = \frac{\epsilon_j{}^{n+1}}{\epsilon_j{}^n} \tag{4.41}$$

The necessary and sufficient condition for the error to remain bounded is that $|G| \leq 1$

Applying the Von Neumann stability method to the unconfined aquifer discretized equation, we can employ that:

$$\frac{S_{i+1}{}^{n+1} - 2S_i{}^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i{}^{n+1}}{\Delta r}\right) = \frac{S}{T}\left(\frac{S_i{}^{n+1} - S_i{}^{n}}{\Delta t}\right) + \alpha S_y \sum_{j=0}^{n-1} \frac{S_i{}^{j+1} - S_i{}^{j}}{\Delta t} \delta^{\alpha}{}_{i,j} \tag{4.42}$$

Expanding

$$\frac{S_{i+1}{}^{n+1} - 2S_i{}^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i{}^{n+1}}{\Delta r}\right) = \frac{S}{T}\left(\frac{S_i{}^{n+1} - S_i{}^{n}}{\Delta t}\right) + S_y \sum_{j=0}^{n-1} \frac{S_i{}^{j+1} - S_i{}^{j}}{\Delta t} \delta^{\alpha}{}_{i,j} + \frac{S_i{}^{n+1} - S_i{}^{n}}{\Delta t} \delta^{\alpha}{}_{i,n} S_y \alpha \tag{4.43}$$

Rearranging

$$\frac{S_{i+1}{}^{n+1} - 2S_i{}^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i{}^{n+1}}{\Delta r}\right) = \frac{S_i{}^{n+1} - S_i{}^{n}}{\Delta t}\left(\frac{S}{T} + S_y\alpha, \delta^{\alpha}{}_{i,j}\right) + S_y \sum_{j=0}^{n-1} \frac{S_i{}^{j+1} - S_i{}^{j}}{\Delta t} \delta^{\alpha}{}_{i,j} \tag{4.44}$$

Factorizing

$$S_i{}^{n+1}\left[\frac{-2}{\Delta r^2} + \frac{1}{r_i}\left(\frac{1}{\Delta r}\right) - \frac{S}{T\Delta t} - S_y\alpha\delta^{\alpha}{}_{i,n}\right] = -S_i{}^{n}\left(\frac{1}{\Delta t}\frac{S}{T} + S_y\alpha\delta^{\alpha}{}_{i,n}\right) - S_{i+1}{}^{n+1}\left[\frac{1}{\Delta r^2} - \frac{1}{r_i}\left(\frac{1}{\Delta r}\right)\right] - S_{i-1}{}^{n+1}\left(\frac{1}{\Delta r^2}\right) + S_y \sum_{j=0}^{n-1} \frac{S_i{}^{j+1} - S_i{}^{j}}{\Delta t} \delta^{\alpha}{}_{i,j} \tag{4.45}$$

Simplifying

$$\propto_1 \left(S_i{}^{n+1}\right) = -\propto_2 \left(S_i{}^{n}\right) - \propto_3 \left(S_{i+1}{}^{n+1}\right) - \propto_4 \left(S_{i-1}{}^{n+1}\right) + S_y \sum_{j=0}^{n-1} \frac{S_i{}^{j+1} - S_i{}^{j}}{\Delta t} \delta^{\alpha}{}_{i,j} \tag{4.46}$$

Note that:

$$\propto_1 = \frac{1}{r_i}\left(\frac{1}{\Delta r}\right) - \frac{S}{T\Delta t} - \propto S_y \delta_{i,n}{}^{\infty} \tag{4.47}$$

$$\propto_2 = \frac{1}{\Delta t}\frac{S}{T} + \propto S_y \delta_{i,n}{}^{\infty} \tag{4.48}$$

$$\propto_3 = \left(\frac{1}{r^2} - \frac{1}{r_i}\left(\frac{1}{\Delta r}\right)\right) \tag{4.49}$$

$$\propto_4 = \left(\frac{1}{\Delta r^2}\right) \tag{4.50}$$

The Von Neumann Stability method can be expressed in the form:

$$\varepsilon_{m(x,t)} = exp[at]exp[ik_m] \tag{4.51}$$

Such that:

$$\varepsilon_j{}^n = \ exp[at]exp[ik_m x] \tag{4.52}$$

$$\varepsilon_j{}^{n+1} = exp[at]exp[ik_m(x+\Delta x)] \tag{4.53}$$

$$\varepsilon_{j+1}{}^{n+1} = \ exp[a(t+\Delta t)]exp[ik_m(x+\Delta x)] \tag{4.54}$$

$$\varepsilon_{j-1}{}^{n-1} = \ exp[a(t-\Delta t)]exp[ik_m(x-\Delta x)] \tag{4.55}$$

From the above discretized equation (4.24), we apply the Von Neumann Stability method to be expressed as:

$$\begin{aligned} &\propto_1 \ exp[a(t+\Delta t)]exp[ik_m x] \\ &= -\propto_2 \ exp[at]exp[ik_m x] \\ &-\propto_3 \ exp[a(t+\Delta t)]exp[ik_m(x+\Delta x)] \\ &-\propto_4 \ exp[a(t+\Delta t)]exp[ik_m(x-\Delta x)] \\ &+ \ S_y \sum_{j=0}^{n-1} \left\{ \frac{exp[a(t+\Delta t)]exp[ik_m x] - exp[at]exp[ik_m x]}{\Delta t} \delta^{\alpha}{}_{i,j} \right\} \end{aligned} \tag{4.56}$$

Taking out $exp[at]exp[ik_m x]$ as a common factor, we have:

$$\begin{aligned} \propto_1 exp[a\Delta t] = -\propto_2 -\propto_3 \ exp[a\Delta t]exp[ik_m \Delta x] +\propto_4 \ exp[a\Delta t]exp[-ik_m \Delta x] \\ + \ S_y \sum_{j=0}^{n-1} \left\{ \frac{exp[(a\Delta t)] - 1}{\Delta t} \delta^{\alpha}{}_{i,j} \right\} \end{aligned} \tag{4.57}$$

Taking out $exp[(a\Delta t)]$ as a common factor, we have:

$$\begin{aligned} exp[(a\Delta t)] \left\{ \propto_1 + \propto_3 \ exp[ik_m \Delta x] - \propto_4 \ exp[-ik_m \Delta x] - \frac{\propto S_y}{\Delta t} \left[\frac{exp[(\Delta tn)]-1}{\Delta t} \right] \right\} \\ = -\propto_2 - \frac{\propto S_y}{\Delta t} \frac{exp[(\Delta tn)]-1}{\Delta t} = -\propto_2 - \frac{\propto S_y}{\Delta t} \frac{exp[(\Delta tn)]-1}{\Delta t} \end{aligned} \tag{4.58}$$

From equation (4.52) and (4.53), we can employ that:

$$\frac{\varepsilon_i{}^{n+1}}{\varepsilon_i{}^n} = \ exp[(a\Delta t)] < 1 \tag{4.59}$$

Expressing the equation in terms of (4.59), we have:

$$exp[(a\Delta t)] = \frac{-\propto_2 - \frac{\propto\ S_y}{\Delta t}\frac{exp[(\Delta tn)]-1}{\Delta t}}{\left\{\propto_1 + \propto_3\ exp[ik_m\Delta x] - \propto_4\ exp[-ik_m\Delta x] - \frac{\propto\ S_y}{\Delta t}\left[\frac{exp[(\Delta tn)]-1}{\Delta t}\right]\right\}} \tag{4.60}$$

If

$$exp[ik_m\Delta x] = Cos[k_m\Delta x] + iSin[k_m\Delta x] \tag{4.61}$$

$$exp[-ik_m\Delta x] = Cos[k_m\Delta x] - iSin[k_m\Delta x] \tag{4.62}$$

Then,

$$exp[(a\Delta t)] = \frac{-\propto_2 - \frac{\propto\ S_y\, exp[(\Delta tn)]-1}{\Delta t}}{\left\{\propto_1 + \propto_3\ (Cos[k_m\Delta x] + iSin[k_m\Delta x]) - \propto_4\ (Cos[k_m\Delta x] - iSin[k_m\Delta x]) - \left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right]\right\}} \tag{4.63}$$

If we express the equation in terms of $exp[(a\Delta t)]$, we can employ that:

$$exp[(a\Delta t)] = \frac{-\propto_2 - \frac{\propto\ S_y\, exp[(\Delta tn)]-1}{\Delta t}}{\left\{\begin{matrix}\propto_1 + \{Cos[k_m\Delta x](\propto_3 - \propto_4)\} \\ -\left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right] + iSin[k_m\Delta x](\propto_3 - \propto_4)\end{matrix}\right\}} \tag{4.64}$$

Since $exp[(a\Delta t)] < 1$, then

$$|exp[(a\Delta t)]| < 1, \left|\frac{-\propto_2 - \frac{\propto S_y\, exp[(\Delta tn)]-1}{\Delta t}}{\begin{matrix}\propto_1 + \{Cos[k_m\Delta x](\propto_3 - \propto_4)\} \\ -\left[\frac{\propto S_y exp[(\Delta tn)]-1}{\Delta t}\right] + iSin[k_m\Delta x](\propto_3 - \propto_4)\end{matrix}}\right| < 1 \tag{4.65}$$

Similarly,

$$\left|\begin{matrix}\propto_1 + \{Cos[k_m\Delta x](\propto_3 - \propto_4)\} \\ -\left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right] + iSin[k_m\Delta x](\propto_3 - \propto_4)\end{matrix}\right| = \sqrt{\begin{pmatrix}\propto_1 + \{Cos[k_m\Delta x](\propto_3 - \propto_4)\} \\ -\left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right]\end{pmatrix}^2 + (iSin[k_m\Delta x](\propto_3 - \propto_4))^2} \tag{4.66}$$

Rearranging

$$\frac{\left|-\propto_2-\frac{\propto\ S_y\ exp[(\Delta tn)]-1}{\Delta t}\right|}{\sqrt{\begin{pmatrix}\propto_1+\{Cos[k_m\Delta x](\propto_3-\propto_4)\}\\-\left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right]\end{pmatrix}^2+(iSin[k_m\Delta x](\propto_3-\propto_4))^2}}<1 \tag{4.67}$$

Simplifying

$$\left|-\propto_2-\frac{\propto\ S_y\ exp[(\Delta tn)]-1}{\Delta t}\right| < \sqrt{\begin{pmatrix}\propto_1+\{Cos[k_m\Delta x](\propto_3-\propto_4)\}\\-\left[\frac{\propto\ S_y exp[(\Delta tn)]-1}{\Delta t}\right]\end{pmatrix}^2+(iSin[k_m\Delta x](\propto_3-\propto_4))^2} \tag{4.68}$$

From the stability analysis performed using the Von Neumann method, it can be concluded that the Delayed yield unconfined response equation is stable, provided that the conditions are met.

4.3 Convergence analysis

The error in a discretization represents the distinction between all the solution of the original real problem and the potential solution of the specific problem that must be characterized in order to make sense and quantify the difference.

Example: The forward difference for $u'(t)$

The estimation error is evaluated with the Taylor series in the forward difference:

$$u'(t_n) \approx [D_t{}^+u]^n = \frac{u^{n+1}-u^n}{\Delta t} \tag{4.69}$$

By writing

$$R^n = [D_t{}^+u]^n - u'(t_n) \tag{4.70}$$

And expanding u^{n+1} in a Taylor series around t_n,

$$u(t_{n+1}) = u(t_n) + u'(t_n)\Delta t + \frac{1}{2}u''^{(t_n)}\Delta t^2 + \ \omega(\Delta t^3) \tag{4.71}$$

The result becomes

$$R = \frac{1}{2}u''(t_n)\Delta t + \ \omega(\Delta t^2) \tag{4.72}$$

Denoting that this is a first order forward difference. Following are the leading concepts of the truncation errors for the first and second order derivatives generally associated with many common finite difference formulae:

$$[D_{2t}u]^n = \frac{u^{n+1} - u^{n-1}}{2\Delta t} = u'(t_n) + R^n \tag{4.73}$$

$$R^n = \frac{1}{6}u'''(t_n)\Delta t^2 + \ \omega(\Delta t^4) \tag{4.74}$$

$$[D_t D_t u]^n = \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} = u''(t_n) + R^n \tag{4.75}$$

$$R^n = \frac{1}{12}u'''(t_n)\Delta t^2 + \ \omega(\Delta t^4) \tag{4.76}$$

$$[D_t{}^+ u]^n = \frac{u^{n+1} - u^n}{\Delta t} = u'(t_n) + R^n \tag{4.77}$$

$$R^n = \frac{1}{2}u''(t_n)\Delta t + \ \omega(\Delta t^2) \tag{4.78}$$

$$\frac{f^{j+1} - f^j}{\Delta t}\int_0^t \frac{1}{2}u''(t_n)\Delta t + \ \omega(\Delta t^2)dt \tag{4.79}$$

$$R^n = \frac{1}{2}u''(t_n)\Delta tt + \ t\omega(\Delta t^2) \tag{4.80}$$

Using the above notation, we can employ that:

$$\begin{aligned}&\frac{S_{i+1}{}^{n+1} - 2S_i{}^{n+1} + S_{i-1}{}^{n+1}}{(\Delta r)^2} + \frac{1}{r_i}\left(\frac{S_{i+1}{}^{n+1} - S_i{}^{n+1}}{\Delta r}\right)\\ &= \frac{S_i{}^{n+1} - S_i{}^n}{\Delta t}\left(\frac{S}{T} + S_y\alpha, \delta^\alpha{}_{i,j}\right) + \ S_y\sum_{j=0}^{n-1}\frac{S_i{}^{j+1} - S_i{}^j}{\Delta t}\delta^\alpha{}_{i,j}\end{aligned} \tag{4.81}$$

By expanding u^{n+1} in a Taylor series around t_n,

$$\begin{aligned}&\frac{1}{6}u'''(t_n)\Delta t^2 + \omega(\Delta t)^4 + \frac{1}{r_i}\left(\frac{1}{2}u''(t_n)\Delta t + \omega(\Delta t^2)\right)\\ &= \frac{S}{T}\left(\frac{1}{2}u''(t_n)\Delta t + \omega(\Delta t^2)\right)\\ &+ \alpha S_y\int_0^t\left(\frac{U^{n+1} - U^n}{\Delta t} + \frac{1}{2}u''(t_n)\Delta t + \omega(\Delta t^2)\right)dt\end{aligned} \tag{4.82}$$

The result becomes

$$\begin{aligned}&\frac{1}{6}u'''(t_n)\Delta t^2 + \omega(\Delta t)^4 + \frac{1}{r_i}\left(\frac{1}{2}u''(t_n)\Delta t + \omega(\Delta t^2)\right)\\ &= \frac{S}{T}\left(\frac{1}{2}u''(t_n)\Delta t + \omega(\Delta t^2)\right) + \alpha S_y\left(\frac{1}{2}u''(t_n)\Delta tt + t\omega(\Delta t^2)\right)\end{aligned} \tag{4.83}$$

From the convergence analysis performed above, we can conclude that the error is of order 4.

CHAPTER FIVE: MODEL WITH STOCHASTIC APPROACH

5.1 Stochastic modelling

Despite comprehensive research in stochastic subsurface hydrology over the past 30 years, the capacity for analysing and modelling heterogeneous groundwater structures continues to remain extremely limited. Though the "stochastic uprising" has generated a vast number of mathematical publications and significantly influenced our thinking about variability, it has had fairly little impact on realistic modelling. In practice today, the prevailing groundwater simulation paradigm is still predominantly deterministic based on merely the same classical conjectures established generations ago.

A crucial question emerges: If heterogeneity is so essential, why is it that no one, in reality uses theories of stochastic modelling (Zhang and Zhang.,2004)? Quite a number of recent reviews made research on this issue in a quite a number of details and came up with the following reasons:

Stochastic coding is likely completely inconsistent with today's conventional new technologies. This is due to the standard raw data are sometimes too restricted to supply the necessary geostatistic variables for stochastic modelling. Relatively new measuring technologies, new data sources with an even much higher resolution and absolutely usable data conversion approaches are required to describe aquifer heterogeneity. However, it is also important to note that it is very difficult to apply stochastic analytical ideas to so many problems of practical complexity. These arguments are based on several restrictive requirements that are useful in practice. The presumptions of ergodicity, stationarity, Gaussian distribution, average uniform flow, and minor disturbance should be relaxed significantly.

Stochastic conjectures are mathematical and complicated and even for experts who have developed them are difficult to implement. A general, integrated computer platform is urgently needed before stochastic modelling can be popularised. Due to these crucial evaluations, we address a number of important conceptual, computational and implementation problems in groundwater modelling in this project. This study represents our attempt to reduce the gap between them.

Stochastic ideas and programs are fundamentally, the practical modelling of groundwater. Stochastic theories of underground flow and transport have also had a major impact on our thinking about uncertainty and heterogeneity. However, the way predictions are obtained and disclosed in practical groundwater modelling studies did not have much impact.

It becomes abundantly clear that stochastic modelling must be made much more general and flexible if it is to become a feasible critical tool. In particular, a stochastic model should be able to immediately integrate site-specific aquifer structures before they can be applied regularly in practice. It must enable the modelling of flexible zones, layers and general trends, as most real-world aquifers not only exhibit "fairly random" heterogeneity but also purposeful "structural" heterogeneity and the statistics portraying aquifer heterogeneity can vary from area to area in reaction to systematic adjustments in the dispersion of aquifer materials.

A vast amount of numerical tactics could also be used to analyse statistically uniform flows and transport, especially inhomogeneous statistical aquifers. These include, for example, Monte Carlo strategies and disturbance methodologies, such as moment equation techniques and second-moment first-order techniques based primarily on Taylor's growth.

All these techniques are, however, computer-intensive when implemented to flow and transport related problems of realistic size, primarily because they still involve the resolution of huge numbers of partial differential equations on some very fine statistical discretizations in order to predict the effect of heterogeneous small dynamics.

5.2 Log-normal distribution

In theory of probability, a log-normal distribution is a continuous statistical probability distribution of a randomly chosen parameter normally distributed by the logarithm. Therefore, if the seemingly random parameter X is dispersed log-normally, $Y = ln(X)$ has a normal distribution. The exponential function of $Y, X = exp(Y)$ also has a log-normal distribution if Y has a normal distribution. A randomly chosen parameter that is dispersed log-normally only takes positive real values.

A log-normal process refers to a probabilistic notion of the multiplier product of many entirely independent, positive random variables. This is enforced by taking into account the central mathematics of the log domain. In addition to that, a log-normal distribution represents the maximum probability of entropy for a randomly chosen variant X specifying the mean and variance of $ln(X)$.

5.2.1 Notation

Given a log-normally distributed random variable X and two parameters, μ and σ that are, respectively, the mean and standard deviation of the variable's natural logarithm, then the logarithm of X is normally distributed, and we can write X as:

$$X = e^{\mu+\sigma Z} \tag{5.1}$$

with Z a standard normal variable.

This relationship is true regardless of the base of the logarithmic or exponential function. If $log_a(Y)$ is normally distributed, then so is $log_b(Y)$, for any two positive numbers $a, b \neq 1$. Likewise, if e^x is log-normally distributed, then so is a^x , where a is a positive number$\neq 1$. The two parameters μ and σ are not location and scale parameters for a log normally distributed random variable X, but they are respectively location and scale parameters for the normally distributed logarithm $ln(X)$. The quantity e^μ is a scale parameter for the family of lognormal distributions.

In contrast, the mean and variance of the non-logarithmized sample values are respectively denoted $m,$ and v in this article. The two sets of parameters can be related as:

$$\mu = ln\left(\frac{m}{\sqrt{1+\frac{v}{m^2}}}\right) \tag{5.2}$$

$$\sigma = ln\left(1+\frac{v}{m^2}\right) \tag{5.3}$$

5.2.2 Probability density function

A positive random variable X is distributed log-normally if the X logarithm is dispersed normally,

$$ln(X) \sim \mathcal{N}(\mu, \sigma^2) \tag{5.4}$$

Let the two functions, Φ and φ, be the cumulative probability distribution function and the density function of the $N(0,1)$ distribution, respectively.

$$f_X(x) = \frac{d}{dx} Pr(X \leq x) = \frac{d}{dx} Pr(lnX \leq lnx) \tag{5.5}$$

$$= \frac{d}{dx}\left(\frac{lnx - \mu}{\sigma}\right) \tag{5.6}$$

$$= \varphi\left(\frac{lnx - \mu}{\sigma}\right)\frac{d}{dx}\left(\frac{lnx - \mu}{\sigma}\right) \tag{5.7}$$

$$= \varphi\left(\frac{lnx - \mu}{\sigma}\right)\frac{d}{dx}\left(\frac{1}{\sigma x}\right) \tag{5.8}$$

$$= \frac{1}{x} \cdot \frac{1}{\sigma\sqrt{2\pi}} exp\left(-\frac{(lnx - \mu)^2}{2\sigma^2}\right) \tag{5.9}$$

5.2.3 Cumulative distributive function

The cumulative distribution function is:

$$f_X(x) = \Phi\left(\frac{lnx - \mu}{\sigma}\right) \tag{5.10}$$

Where Φ depicts the cumulative distribution function of the standard normal distribution (i.e. $N(0,1)$).

This can also be denoted as follows:

$$\frac{1}{2}\left[1 + erf\left(\frac{lnx - \mu}{\sigma\sqrt{2}}\right)\right] = \frac{1}{2} erfc\left(\frac{lnx - \mu}{\sigma\sqrt{2}}\right) \tag{5.11}$$

The following figures illustrate semi log-normal density functions and a cumulative distribution function of the log-normal distribution.

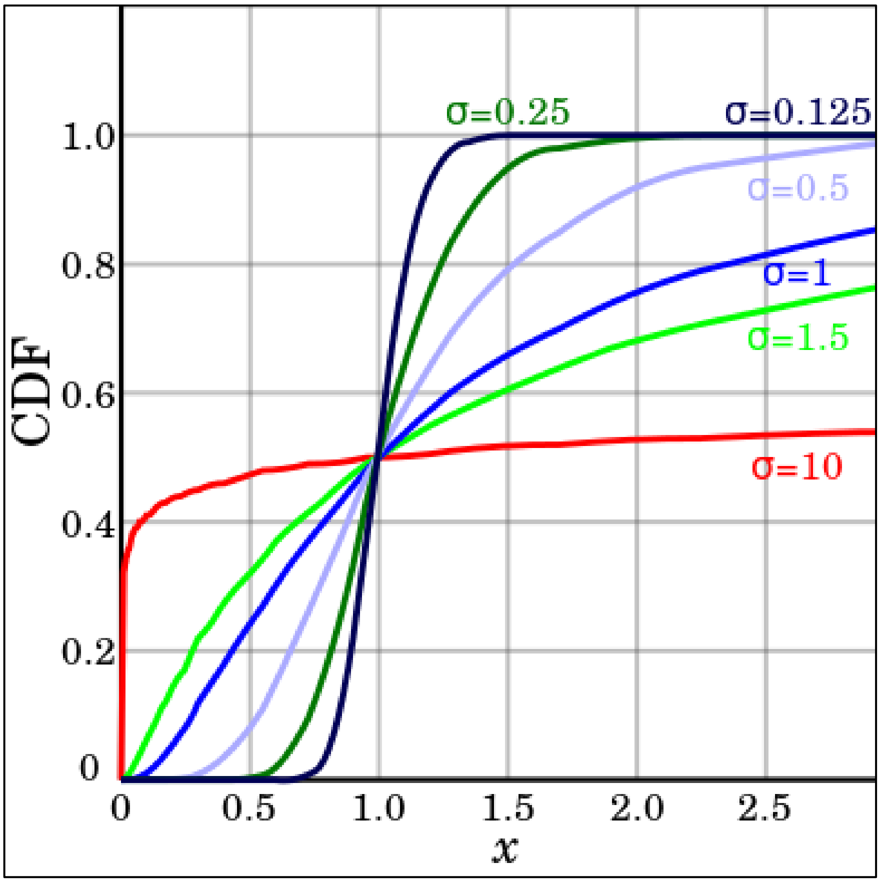

Figure 7: Some log-normal density functions with identical parameter μ but differing parameters σ (Lohman, 1972)

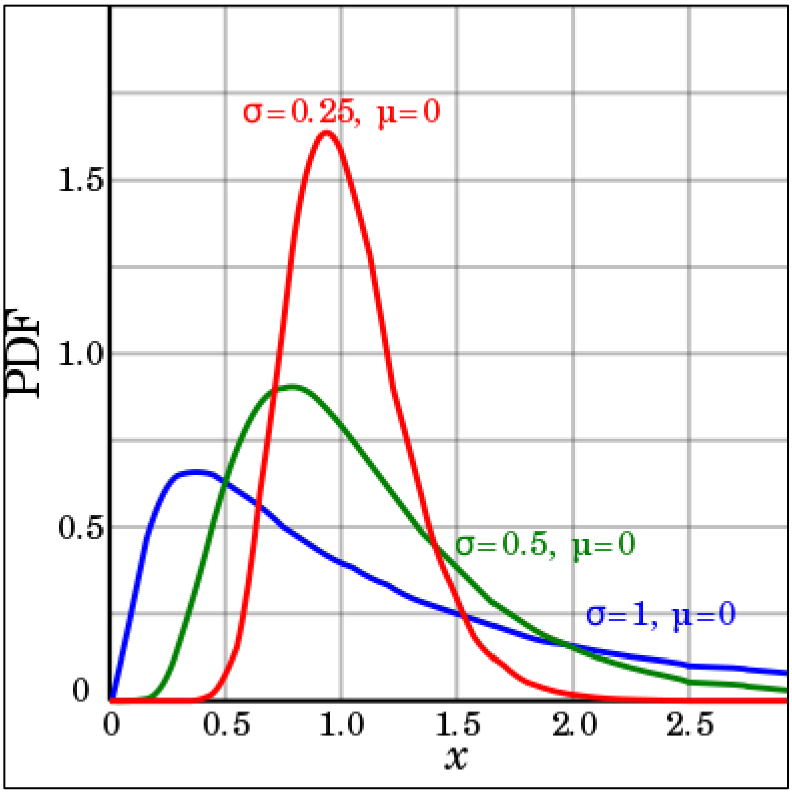

Figure 8: Cumulative distribution function of the log-normal distribution (with $\mu = 0$) (Lohman, 1972)

5.2.4 Mean

The population mean or expected value in probability and statistics is a measure of the central trend either of the probability distribution or of the random variable characterized by that particular distribution. For instance, in a discrete distribution of the probability of a random variable X , the mean is equivalent to the sum over each possible value weighted by the probability of that value; i.e., it is calculated by taking the product of each possible value x of X and its probability (x) . By summing up all these products together, the result becomes $\mu = \sum xp(x)$. But not every distribution of probabilities has a delineated mean;

For a relatively limited population, the mean population of a property is entirely equal to the arithmetic mean of the property as each member of the population is considered. The population mean height, for example, is equal to the sum of the heights of each person divided by the total number of persons. The mean sample may differ from the mean population, in particular in small samples. The law of large numbers states that the larger the sample size, the more likely the mean of the sample is to be close to the mean of the population.

Arithmetic mean (AM)

The arithmetic mean of a sample, usually referred to as average, is the sum of all the sampled values divided by the total number of samples

$$\bar{x} = \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right) = \frac{x_1 + x_2 + \ldots x_n}{n} \qquad (5.12)$$

5.2.5 Variance and standard deviation

Variance is the implication of the square deviation of a completely random variable from its mean in probability theory and statistics. Constructively, it measures the distance between a pair of (random) numbers and their average value, see figure 9. Variance has a key role in statistics, where parameter estimation, statistical inference, theory tests, fitness and Monte Carlo sampling are some of the ideas used. Variance is an important research tool in which statistical data analysis is prevalent. The variance can be calculated by squaring the standard deviation and it is frequently symbolised by σ^2 ,s^2 , or $Var(X)$.

So, taking note that $\bar{x}$ is the mean, $x_1 + x_2 + \ldots x_n$ depicting the sum of all samples and n representing the number of samples, we can employ that the variance can be denoted as:

$$\sigma^2 = \frac{(x_1 - \bar{x}) + (x_2 - \bar{x}) + \ \ldots (x_n - \bar{x})}{n} \tag{5.13}$$

$$\sigma^2 = \frac{(x_1 - \bar{x})^2 + \ (x_1 - \bar{x})^2 + \cdots (x_n - \bar{x})^2}{n} \tag{5.14}$$

$$\sigma^2 = \frac{\sum (x - \bar{x})^2}{n} \tag{5.15}$$

Standard deviation can thus be denoted as:

$$\sigma = \sqrt{\frac{(x_1 - \bar{x})^2 + \ (x_1 - \bar{x})^2 + \cdots (x_n - \bar{x})^2}{n}} \tag{5.16}$$

$$\sigma = \sqrt{\frac{\sum (x - \bar{x})^2}{n}} \tag{5.17}$$

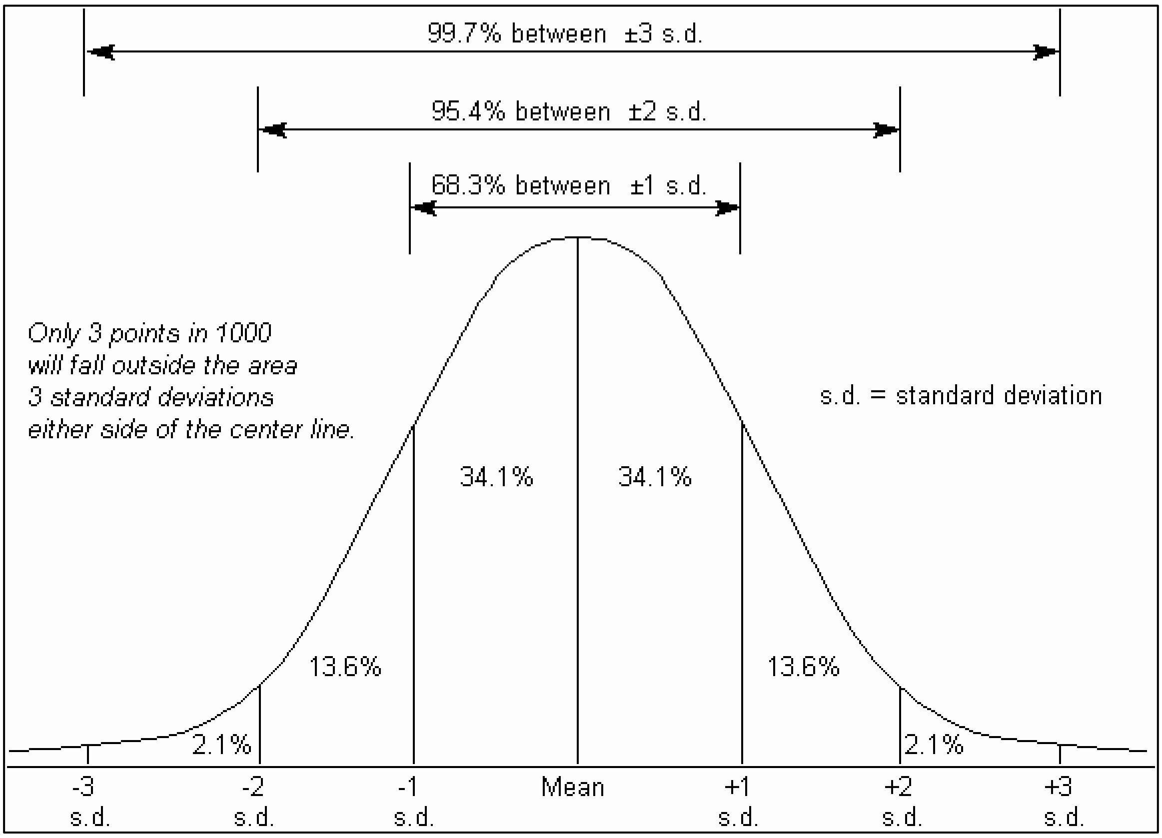

Figure 9: Graphical representation of the standard deviation and average (Salkind, 2010)

5.3 The stochastic model

By varying aquifer parameters, we develop the stochastic model. From our defined unconfined aquifer equation from chapter one, i.e., equation (1.6), all the parameters including Storativity, Transmissivity, Specific yield and the delay index are varied, through which a mean will be calculated with the aim of developing a stochastic model, through which analysis will be made from.

$$\frac{\partial^2 s^*}{\partial r^2}+\frac{1}{r}\frac{\partial s^*}{\partial r}=\left[\frac{S}{T}\frac{\partial s^*}{\partial t}\right]+\left\{\alpha S_y\int_0^t\frac{\partial s^*}{\partial \tau}e^{-\alpha(t-\tau)}d\tau\right\} \tag{5.18}$$

Introducing the stochastic component

$$\frac{\partial^2 s^*}{\partial r^2}+\frac{1}{r}\frac{\partial s^*}{\partial r}=\frac{\bar{S}\ +\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)}{\bar{T}\ +\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)}\frac{\partial s}{\partial t}$$
$$+\alpha\overline{S_y}\,\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)\int_0^t\frac{\partial s}{\partial \tau}exp[-\alpha(t-\tau)]d_\tau \tag{5.19}$$

After descretization using Forward Euler method, we have:

$$\frac{S_{i+1}^{n+1}-2S_i^{\ n+1}+S_{i-n}^{n+1}}{(\Delta r)^2}+\frac{1}{r_i}\left(\frac{S_{i+1}^{n+1}-S_i^{\ n+1}}{\Delta r}\right)$$
$$=\frac{\bar{S}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)}{\bar{T}\ +\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)}\left(\frac{S_i^{\ n+1}-S_i^{\ n}}{\Delta t}\right)+\ \alpha\overline{S_y}$$
$$+\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)\sum_{j=0}^{n}\frac{S_i^{\ j+1}-S_i^{\ j}}{\Delta t}\frac{1+e^{-\Delta t}}{\alpha}\left\{\left[\frac{exp\left[\Delta t(n-j)-exp[\Delta t(n-j-1)]\right]}{\alpha}\right]\right\}$$

(5.20)

$$\frac{S_{i+1}^{n+1}-2S_i^{\ n+1}+S_{i-n}^{n+1}}{(\Delta r)^2}+\frac{1}{r_i}\left(\frac{S_{i+1}^{n+1}-S_i^{\ n+1}}{\Delta r}\right)$$
$$=\frac{\bar{S}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)}{\bar{T}\ +\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)}\left(\frac{S_i^{\ n+1}-S_i^{\ n}}{\Delta t}\right)+\ \alpha\overline{S_y} \tag{5.21}$$
$$+\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)\sum_{j=0}^{n}\frac{S_i^{\ j+1}-S_i^{\ j}}{\Delta t}\frac{1+e^{-\Delta t}}{\alpha}\delta_{j,n}^{\alpha}$$

Where $\delta_{j,n}^{\alpha}=\frac{1+e^{-\Delta t}}{\alpha}\left\{\left[\frac{exp\left[\Delta t(n-j)-exp[\Delta t(n-j-1)]\right]}{\alpha}\right]\right\}$ (5.22)

5.3.1 Von Neumann Stability analysis

$$\frac{S_{i+1}^{n+1}-2S_i{}^{n+1}+S_{i-n}^{n+1}}{(\Delta r)^2}+\frac{1}{r_i}\left(\frac{S_{i+1}^{n+1}-S_i{}^{n+1}}{\Delta r}\right)$$

$$=\frac{\bar{S}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)}{\bar{T}\ +\lambda\frac{1}{x}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnx-\mu)^2}{2\sigma^2}\right)}\left(\frac{S_i{}^{n+1}-S_i{}^{n}}{\Delta t}\right)+\ \alpha\overline{S_y}$$

$$+\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)\sum_{j=0}^{n}\frac{S_i{}^{j+1}-S_i{}^{j}}{\Delta t}\frac{1+e^{-\Delta t}}{\alpha}\left\{\left[\frac{exp\big[\Delta t(n-j)-exp[\Delta t(n-j-1)]\big]}{\alpha}\right]\right\}$$

(5.23)

We let:

$$\bar{S}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)=S_i \tag{5.24}$$

$$\bar{T}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)=T_i \tag{5.25}$$

$$\overline{S_y}\ +\lambda\frac{1}{r_i}.\frac{1}{\sigma\sqrt{2\pi}}exp\left(\frac{-(lnr_i-\mu)^2}{2\sigma^2}\right)=S_{y_i}$$

(5.26)

Simplifying

$$\frac{S_{i+1}^{n+1}-2S_i{}^{n+1}+S_{i-n}^{n+1}}{(\Delta r)^2}+\frac{1}{r_i}\left(\frac{S_{i+1}^{n+1}-S_i{}^{n+1}}{\Delta r}\right)$$

$$=\frac{S_i}{T_i}\left(\frac{S_i{}^{n+1}-S_i{}^{n}}{\Delta t}\right)+\ \alpha S_y\sum_{j=0}^{n=1}\frac{S_i{}^{j+1}-S_i{}^{j}}{\Delta t}\delta_{i,j}^{\alpha} \tag{5.27}$$

$$+\frac{S_i{}^{n+1}-S_i{}^{n}}{\Delta t}\delta_{n,j}^{\alpha}S_y\alpha$$

Grouping

$$\frac{S_{i+1}^{n+1}-2S_i{}^{n+1}+S_{i-n}^{n+1}}{(\Delta r)^2}+\frac{1}{r_i}\left(\frac{S_{i+1}^{n+1}-S_i{}^{n+1}}{\Delta r}\right)$$

$$=\left(\frac{S_i{}^{n+1}-S_i{}^{n}}{\Delta t}\right)\left(\frac{S_i}{T_i}+S_{y_i}\alpha\delta_{n,j}^{\alpha}\right)+\ \alpha S_y\sum_{j=0}^{n-1}\frac{S_i{}^{j+1}-S_i{}^{j}}{\Delta t}\delta_{i,j}^{\alpha} \tag{5.28}$$

Factorising

$$S_i{}^{n+1}\left[\frac{-2}{\Delta r^2}+\frac{1}{r_i}\left(\frac{1}{\Delta r}\right)-\frac{S}{T\Delta t}-S_y\alpha\delta^{\alpha}{}_{i,n}\right]= \tag{5.29}$$

$$-S_i{}^{n}\left(\frac{1}{\Delta t}\frac{S}{T}+S_y\alpha\delta^{\alpha}{}_{i,n}\right)-S_{i+1}{}^{n+1}\left[\frac{1}{\Delta r^2}-\frac{1}{r_i}\left(\frac{1}{\Delta r}\right)\right]-S_{i-1}{}^{n+1}\left(\frac{1}{\Delta r^2}\right)$$

$$+\alpha S_y\textstyle\sum_{j=0}^{n-1}\frac{S_i{}^{j+1}-S_i{}^{j}}{\Delta t}\delta^{\alpha}{}_{i,j}$$

Applying the Von Neumann Stability notation

$$\delta_{n+1}e^{ikmx}(\alpha_1) = \delta_n e^{ikmx}(\alpha_2) - \delta_{n+1}e^{ikmx}e^{ikm\Delta x}(\alpha_3) - \delta_{n+1}e^{ikmx}e^{-ikm\Delta x}(\alpha_4) + \alpha S_y \sum_{j=0}^{n-1} \delta_{n-j}\frac{e^{ikmx}e^{ikm\Delta x} - e^{ikmx}}{\Delta t}\delta_{n,j} \tag{5.30}$$

Note that:

$$\alpha_1 = \left[\frac{-2}{\Delta r^2} + \frac{1}{r_i}\left(\frac{1}{\Delta r}\right) - \frac{S}{T\Delta t} - S_y \alpha \delta^{\alpha}{}_{i,n}\right] \tag{5.31}$$

$$\alpha_2 = \left(\frac{1}{\Delta t}\frac{S}{T} + S_y \alpha \delta^{\alpha}{}_{i,n}\right) \tag{5.32}$$

$$\alpha_3 = \left[\frac{1}{\Delta r^2} - \frac{1}{r_i}\left(\frac{1}{\Delta r}\right)\right] \tag{5.33}$$

$$\alpha_4 = \left(\frac{1}{\Delta r^2}\right) \tag{5.34}$$

$$\delta_{n+1}e^{ikmx}(\alpha_1) = \delta_n e^{ikmx}(\alpha_2) - \delta_{n+1}e^{ikmx}e^{ikm\Delta x}(\alpha_3) - \delta_{n+1}e^{ikmx}e^{-ikm\Delta x}(\alpha_4) + \alpha S_y \sum_{j=0}^{n-1} \delta_{n-j}\frac{e^{ikmx}e^{ikm\Delta x} - e^{ikmx}}{\Delta t}\delta_{n,j} \tag{5.35}$$

Dividing by e^{ikmx} , we get:

$$\delta_{n+1}(\alpha_1) = \delta_n(\alpha_2) - \delta_{n+1}e^{ikm\Delta x}(\alpha_3) - \delta_{n+1}e^{-ikm\Delta x}(\alpha_4) + \alpha S_y \sum_{j=0}^{n-1} \delta_{n-j}\left(\frac{e^{ikm\Delta x}}{\Delta t}\right) \tag{5.36}$$

Grouping

$$\delta_{n+1}\left(\alpha_1 - \alpha_3 e^{ikm\Delta x} - e^{-ikm\Delta x}\alpha_4\right) = \delta_n(\alpha_2) + \alpha S_y \sum_{j=0}^{n-1} \delta_{n-j}\delta_{n,j} \tag{5.37}$$

If

$$exp[ik_m\Delta x] = Cos[k_m\Delta x] + iSin[k_m\Delta x] \tag{5.38}$$

$$exp[-ik_m\Delta x] = Cos[k_m\Delta x] - iSin[k_m\Delta x] \tag{5.39}$$

Then

$$\delta_{n+1}\left(\alpha_1 - \alpha_3\big(Cos(ikm\Delta x) + iSin(ikm\Delta x)\big) - \alpha_4\big(Cos(ikm\Delta x) + iSin(ikm\Delta x)\big)\right) = \delta_n(\alpha_2) + \alpha S_y \sum_{j=0}^{n-1} \delta_{n-j}\delta_{n,j} \tag{5.40}$$

We prove the stability via induction technique when $n = 0$

$$\delta_1\{\alpha_1 - Cos(ikm\Delta x)(\alpha_4 + \alpha_3) + iSin(ikm\Delta x)(\alpha_4 - \alpha_3)\} = \delta_0\alpha_2 \tag{5.41}$$

Resulting

$$\left|\frac{\delta_1}{\delta_0}\right| < 1 \to \frac{\alpha_2}{\alpha_1 - Cos(ikm\Delta x)(\alpha_4 + \alpha_3) + iSin(ikm\Delta x)(\alpha_4 - \alpha_3)} < 1 \tag{5.42}$$

Which is time in general, so we assume that for all $n \geq 0$

$$\left|\frac{\delta_n}{\delta_0}\right| < 1 \tag{5.43}$$

We want to prove that

$$\left|\frac{\delta_{n+1}}{\delta_0}\right| < 1 \tag{5.44}$$

But

$$\delta_{n+1} = \frac{\alpha_2}{\varphi}\delta_n + \sum_{j=0}^{n-1}\frac{\alpha S_{y\delta_{n,j}}}{\varphi} \tag{5.45}$$

$$|\delta_{n+1}| = \left|\frac{\alpha_2}{\varphi}\delta_n + \sum_{j=0}^{n-1}\frac{\alpha S_{y\delta_{n,j}\delta_{n-j}}}{\varphi} \leq \left|\frac{\alpha_2}{\varphi}\right||\delta_n| + \sum_{j=0}^{n-1}\left|\frac{\alpha S_{y\delta_{n,j}}}{\varphi}\right||\delta_{n-j}|\right| \tag{5.46}$$

From inductive principle, we have

$$|\delta_{n+1}| < \left|\frac{\alpha_2}{\varphi}\right||\delta_0| + \sum_{j=0}^{n-1}\left|\frac{\alpha S_{y\delta_{n,j}}}{\varphi}\right||\delta_0| \tag{5.47}$$

$$|\delta_{n+1}| < |\delta_0|\left|\left(\frac{\alpha_2}{\varphi} + \sum_{j=0}^{n-1}\frac{\alpha S_{y\delta_{n,j}}}{\varphi}\right)\right| \tag{5.48}$$

$$\left|\frac{\delta_{n+1}}{\delta_0}\right| < \left|\frac{\alpha_2}{\varphi} + \sum_{j=0}^{n-1}\frac{\alpha S_{y\delta_{n,j}}}{\varphi}\right| \tag{5.49}$$

$$\left|\frac{\delta_{n+1}}{\delta_0}\right| < 1 \to \alpha_2 + \sum_{j=0}^{n-1}\alpha\, S_{y\delta_{n,j}} < \varphi \tag{5.50}$$

From the stability analysis performed above using the inductive principle, we can conclude that the equation is stable, provided that the conditions are met.

CHAPTER SIX: NEW NUMERICAL SCHEME: LAGRANGE POLYNOMIAL INTERPOLATION AND THE TRAPEZOIDAL RULE

6.1 Lagrange polynomial interpolation and the trapezoidal rule

For the past decades, multiple numerical methods have been established to resolve partial differential equations that entail integrals as well as derivatives. To mention a few, Crank and Nicholson merged the forward and backward method to produce a numerical scheme that is used to discretise partial differential equations and seems to be very stable. Although these numerical schemes are still used to date, new numerical schemes are constantly established to solve differential equations based on the complexity of the problem. For instance, Adam and Bashforth established an advanced numerical scheme employing the Lagrange polynomial interpolation. Additionally, Atangana and Batogna established a new numerical scheme employing the Laplace transform as well as the Adam-Bashforth procedure. All these new numerical schemes that are constantly established are still used to date. These numerical schemes however have limitations and as a result, more advanced numerical schemes are still appreciated. In this unit, we employ a new numerical scheme that integrates the Lagrange polynomial interpolation as well as the trapezoidal rule. Using this numerical scheme on the following partial differential equation, we can employ that:

$$\frac{\partial^2 s^*}{\partial r^2}+\frac{1}{r}\frac{\partial s^*}{\partial r}=\left[\frac{S}{T}\frac{\partial s^*}{\partial t}\right]+\left\{\alpha S_y\int_0^t\frac{\partial s^*}{\partial \tau}e^{-\alpha(t-\tau)}d\tau\right\} \tag{6.1}$$

$$\frac{\partial s}{\partial t}=\frac{T}{S}\left(\frac{\partial^2 s}{\partial r^2}+\frac{1}{r}\frac{\partial s}{\partial r}-\alpha S_y\int_0^t\frac{\partial s}{\partial \tau}e^{-\alpha(t-\tau)}d\tau\right) \tag{6.2}$$

$$\frac{\partial s}{\partial t}=f(S,r,t)+\int_0^t F(S,r,\tau)d_t \tag{6.3}$$

Where

$$f(S,r,t)=\frac{T}{S}\left(\frac{\partial^2 s}{\partial r^2}+\frac{1}{r}\frac{\partial s}{\partial r}\right) \tag{6.4}$$

$$F(S,r,t)d_t=-\frac{T}{S}\alpha S_y\left(\int_0^t\frac{\partial s}{\partial \tau}e^{-\alpha(t-\tau)}d\tau\right) \tag{6.5}$$

This equation is an integro-differential equation

$$\int_0^t\frac{\partial s}{\partial \tau}d\tau=\int_0^t f(S,r,t)d_\tau+\int_0^t\int_0^\tau F(S,r,l)d_l d_\tau \tag{6.6}$$

$$S(r,t)-S(r,0)=\int_0^t f(S,r,\tau)+\int_0^t\int_0^\tau F(S,r,l)d_l d_\tau \tag{6.7}$$

At the point $t = t_{n+1}$, we have

$$S(r, t_{n+1}) - S(r, 0) = \int_0^{t_{n+1}} f(S, r, t) d_\tau + \int_0^{t_{n+1}} \int_0^t F(S, r, l) d_l d_\tau \tag{6.8}$$

Also at

$$t = t_n \tag{6.9}$$

$$S(r, t_n) - S(r, 0) = \int_0^{t_n} f(S, r, t) d_t + \int_0^{t_n} \int_0^t F(S, r, l) d_l d_t \tag{6.10}$$

$$(6.8) - (6.10)$$

$$S(r, t_{n+1}) - S(r, t_n) = \int_0^{t_{n+1}} f(S, r, t) d_t + \int_0^{t_{n+1}} \int_0^t F(S, r, l) d_l d_t \tag{6.11}$$

We know that using Lagrange polynomial

$$\int_a^b f(t) d_t = \frac{3}{2}(b - a)\, f(b) - \frac{(b - a)}{2} f(a) \tag{6.12}$$

$$\int_{t_n}^{t_{n+1}} f(S, r, t) d_t = \frac{3(t_{n+1} - t_n)}{2} f(S, r, t_n) - \frac{(t_{n+1} - t_n)}{2} f(S, r, t_{n-1}) \tag{6.13}$$

$$\int_{t_n}^{t_{n+1}} f(S, r, t) d_t = \frac{3(\Delta t)}{2}\, f(S^n, r, t_n) - \frac{\Delta t}{2} f(S^{n-1}, r, t_{n-1}) \tag{6.14}$$

$$\int_{t_n}^{t_{n+1}} \int_0^t F(S, r, l) d_l d_t = \int_{t_n}^{t_{n+1}} g(t) d_t \tag{6.15}$$

$$\int_a^b g(t) d_t = \frac{(b - a)}{2} [f(b) + f(a)] \tag{6.16}$$

$$\int_{t_n}^{t_{n+1}} g(t) d_t = \frac{(t_{n+1} - t_n)}{2} [g(t_{n+1}) + g(t_n)] \tag{6.17}$$

$$= \frac{\Delta t}{2}\left[\int_0^{t_{n+1}} F(S, r, \tau) d_\tau + \int_0^{t_n} F(S, r, \tau) d_\tau\right]$$

$$= \frac{\Delta t}{2}\left[\int_0^{t_n} F(S, r, \tau) d_\tau + \int_{t_n}^{t_{n+1}} F(S, r, \tau) d_\tau + \int_0^{t_n} F(S, r, \tau) d_\tau\right] \tag{6.18}$$

$$= \frac{\Delta t}{2}\left[2\int_0^{t_n} F(S, r, \tau) d_\tau + \int_{t_n}^{t_{n+1}} F(S, r, \tau) d_\tau\right] \tag{6.19}$$

$$\begin{aligned} = \frac{\Delta t}{2}\Bigg[2\int_0^{t_1} F(S, r, \tau) d_\tau + 2\int_{t_1}^{t_n} F(S, r, \tau) d_\tau + \frac{3}{2}\Delta t\, F(S^n, r, t_n) \\ - \frac{\Delta t}{2} F(S^{n-1}, r, t_{n-1})\Bigg] \end{aligned} \tag{6.20}$$

$$\begin{aligned} = \frac{\Delta t}{2}\Bigg[\frac{2\Delta t}{2}\Bigg(\big(F(S^1, r, t_1) + F(S^0, r, t_0)\big) + \frac{3}{2}\Delta t\, F(S^n, r, t_n) \\ - \frac{\Delta t}{2}\, F(S^{n-1}, r, t_{n-1}) + 2\sum_{j=1}^{n-1} \int_{t_j}^{t_{j+1}} F(S, r, t) d_t = \Bigg)\Bigg] \end{aligned} \tag{6.21}$$

$$= \frac{\Delta t}{2}\left\{\Delta t\left[F(S^{1,}r,t_1) + F(S^0,r,t_0) + \frac{3}{2}\Delta t\, F(S^n,r,t_n) - \frac{\Delta t}{2}F(S^{n-1},r,t_{n-1}) + 2\sum_{j=1}^{n-1}\left[\frac{3}{2}\Delta t\, F\left(S^j,r,t_j\right) - \frac{\Delta t}{2}F\left(S^{j-1},r,t_{j-1}\right)\right]\right]\right\} \tag{6.22}$$

$$S(r,t_{n+1}) - S(r,t_n) \tag{6.23}$$

$$= \frac{3}{2}\Delta t\, f(S^n,r,t_n) - \frac{\Delta t}{2}f(S^{n-1},r,t_{n-1}) + \frac{(\Delta t)^2}{2}\left(F(S^1,r,t_1) - F(S^0,r,t_0)\right) + \frac{3}{4}\Delta t^2 F(S^n,r,t_n) - \frac{(\Delta t)^2}{4}F\,(S^{n-1},r,t_{n-1}) + \sum_{j=1}^{n-1}\left[\frac{3}{2}(\Delta t)^2 F\left(S^j,r,t_j\right) - \frac{(\Delta t)^2}{2}F\left(S^{j-1},r,t_{j-1}\right)\right] \tag{6.24}$$

Now we discretise in space to have:

At $r = r_i$, we have

$$S_i^{n+1} - S_i^n = \frac{3}{2}\Delta t\, f(S_i^n,r_i,t_n) - \frac{\Delta t}{2}\, f(S_i^{n-1},r_i,t_{n-1}) + \frac{(\Delta t)^2}{2}\left[F(S_i^1,r_i,t_1) - F(S_i^0,r_i,t_0)\right] + \frac{3}{4}(\Delta t)^2 F(S_i^n,r_i,t_n) - \frac{(\Delta t)^2}{4}\, F\,(S_i^{n-1},r_i,t_{n-1}) + \sum_{j=1}^{n-1}\left[\frac{3}{2}(\Delta t)^2 F\left(S_i^j,r_i,t_j\right) - \boxed{\frac{(\Delta t)^2}{2}} F\left(S_i^{j-1},r_i,t_{j-1}\right)\right] \tag{6.25}$$

Now we discretise in time to have

$$f(S,r,t) = \frac{T}{S}\left(\frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r}\right) \tag{6.26}$$

$$f(S_i^1,r_i,t_i) = \frac{T}{S}\left[\frac{S_{i+1}^1 - 2S_i^1 + S_{i-1}^1}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^1 - S_{i-1}^1}{\Delta x}\right] \tag{6.27}$$

$$F(S,r,t) = -\frac{T}{S}\alpha S_y\left(\frac{\partial s}{\partial t}e^{-\alpha(t-\tau)}\right) \tag{6.28}$$

$$F\left(S_i^1,r_i,t_j\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^1 - S_i^0}{\Delta t}e^{-\alpha(t_1-t_0)}\right) \tag{6.29}$$

$$f\left(S_i^n,r_i,t_j\right) = \frac{T}{S}\left[\frac{S_{i+1}^n - 2S_i^n + S_{i-1}^n}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^n - S_{i-1}^n}{\Delta x}\right] \tag{6.30}$$

$$F\left(S_i^n,r_i,t_j\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^n - S_i^0}{\Delta t}e^{-\alpha(t_n-t_0)}\right) \tag{6.31}$$

$$f\left(S_i^{n-1}, r_i, t_j\right) = \frac{T}{S}\left[\frac{S_{i+1}^{n-1} - 2S_i^{n-1} + S_{i-1}^{n-1}}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^{n-1} - S_{i-1}^{n-1}}{\Delta x}\right] \tag{6.32}$$

$$F\left(S_i^{n-1}, r_i, t_j\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^{n-1} - S_i^0}{\Delta t}e^{-\alpha\left(t_{n-1}-t_j\right)}\right) \tag{6.33}$$

$$f(S_i^0, r_i, t_i) = \frac{T}{S}\left[\frac{S_{i+1}^0 - 2S_i^0 + S_{i-1}^0}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^0 - S_{i-1}^0}{\Delta x}\right] \tag{6.34}$$

$$F\left(S_i^0, r_i, t_j\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^{0-1} - S_i^0}{\Delta t}\right) \tag{6.35}$$

$$\left(S_i^j, r_i, t_j\right) = \frac{T}{S}\left[\frac{S_{i+1}^j - 2S_i^j + S_{i-1}^j}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^j - S_{i-1}^j}{\Delta x}\right] \tag{6.36}$$

$$F\left(S_i^j, r_i, t_j\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^j - S_i^0}{\Delta t}e^{-\alpha\left(t_n-t_j\right)}\right) \tag{6.37}$$

$$\left(S_i^{j-1}, r_i, t_{j-1}\right) = \frac{T}{S}\left[\frac{S_{i+1}^{j-1} - 2S_i^{j-1} + S_{i-1}^{j-1}}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^{j-1} - S_{i-1}^{j-1}}{\Delta x}\right] \tag{6.38}$$

$$F\left(S_i^{j-1}, r_i, t_{j-1}\right) = -\frac{T}{S}\alpha S_y\left(\frac{S_i^{j-1} - S_i^0}{\Delta t}e^{-\alpha\left(t_n-t_{j-1}\right)}\right) \tag{6.39}$$

$$\begin{aligned}
S_i^{n+1} - S_i^n = {} & \frac{3}{2}\Delta t\ \left[\frac{T}{S}\left[\frac{S_{i+1}^n - 2S_i^n + S_{i-1}^n}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^n - S_{i-1}^n}{\Delta x}\right]\right] \\
& - \frac{\Delta t}{2}\left[\frac{T}{S}\left[\frac{S_{i+1}^{n-1} - 2S_i^{n-1} + S_{i-1}^{n-1}}{(\Delta x)^2} + \frac{1}{r_i}\frac{S_{i+1}^{n-1} - S_{i-1}^{n-1}}{\Delta x}\right]\right] \\
& + \frac{(\Delta t)^2}{2}\left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^1 - S_i^0}{\Delta t}e^{-\alpha(t_1-t_0)}\right)\right. \\
& \left. - \left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^{0-1} - S_i^0}{\Delta t}e^{-\alpha\left(t_n-t_j\right)}\right)\right]\right] \\
& + \frac{3}{4}(\Delta t)^2\left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^n - S_i^0}{\Delta t}e^{-\alpha(t_n-t_0)}\right)\right] \\
& - \frac{(\Delta t)^2}{4}\ \left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^{n-1} - S_i^0}{\Delta t}e^{-\alpha(t_{n-1}-t_0)}\right)\right] \\
& + \sum_{j=1}^{n-1}\left[\frac{3}{2}(\Delta t)^2\left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^j - S_i^0}{\Delta t}e^{-\alpha\left(t_j-t_0\right)}\right)\right]\right. \\
& \left. - \frac{(\Delta t)^2}{2}\ \left[-\frac{T}{S}\alpha S_y\left(\frac{S_i^{j-1} - S_i^0}{\Delta t}e^{-\alpha\left(t_{j-1}-t_0\right)}\right)\right]\right]
\end{aligned} \tag{6.40}$$

This newly derived numerical scheme uses Lagrange polynomial interpolation and the trapezoidal rule to discretise in space and time.

CHAPTER SEVEN: NUMERICAL SIMULATIONS

A Matlab software approach is used to simulate the flow of groundwater in graphic form. Matlab is a MathWorks, Inc., Natick, USA software. The operating system was mainly used only for mathematical calculation, facilitating computed matrix equations and their systems to be calculated. All significant parameters can use the matrix as input directly. From that year onwards, the software is still being developed and the area of the users is increasing each year. Matlab has become the legal standard in the field of simulation and modelling and it has been used primarily in mathematics, statistics and several other professions by researchers and students in academic institutions. Matlab has several advantages compared with other software like Mathematica or Maple. To name a few, its open architecture allows all source code to be shared between the user community and several different areas are solved and the solution usually appears as a new tool box.

In this section, we will first show simulations from the deterministic approach, were all aquifer parameters are kept constant. Contrary to that is the stochastic approach, were aquifer parameters are varied. We present below the numerical simulations of the mathematical model for different values of stochastic parameters.

The numerical results are depicted in figures 10 to 23. The figures simulate change in water level and their respective contour plots. The initial conditions and boundary conditions used to simulate the following models are depicted in the appendix. The aquifer parameters were varied for each simulation. The transmissivity of the aquifer ranged between 400 to 800m^2/d, the specific yield ranged between 0.0001, to 0.38, the storativity of course between 0.001 to 0.009, we assumed the initial level of water to be 2, lastly, the delay index varied from 0.001 to 6.

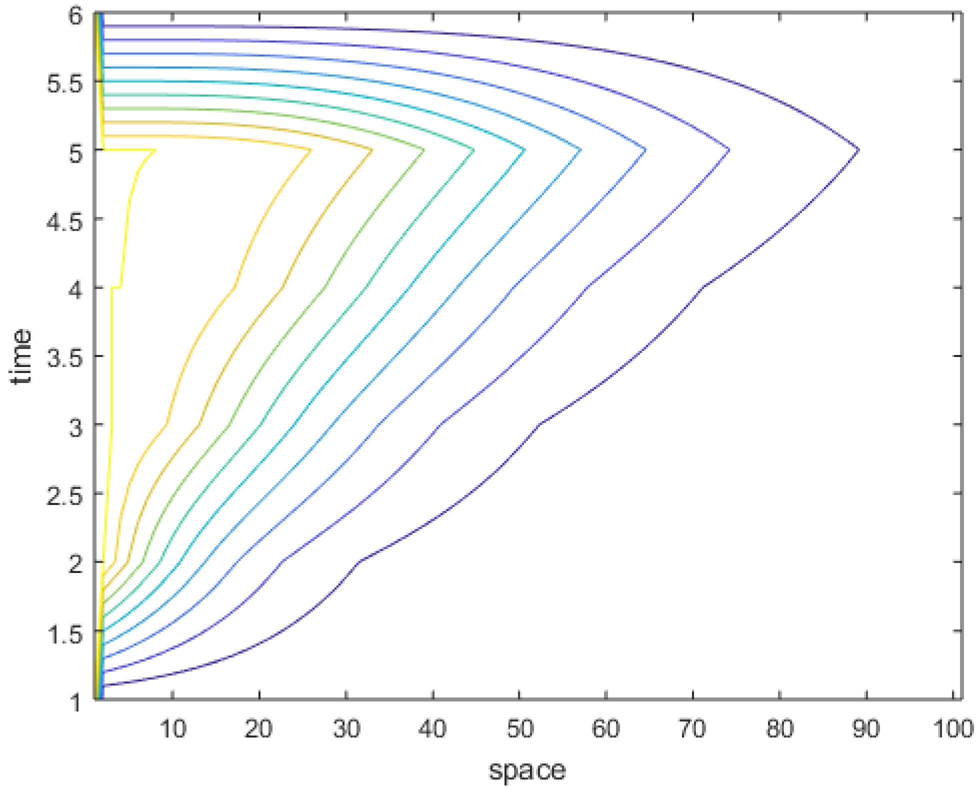

Figure 10: Contour plot solution for delay constant 3, average transmissivity T =405, specific yield =0. 002

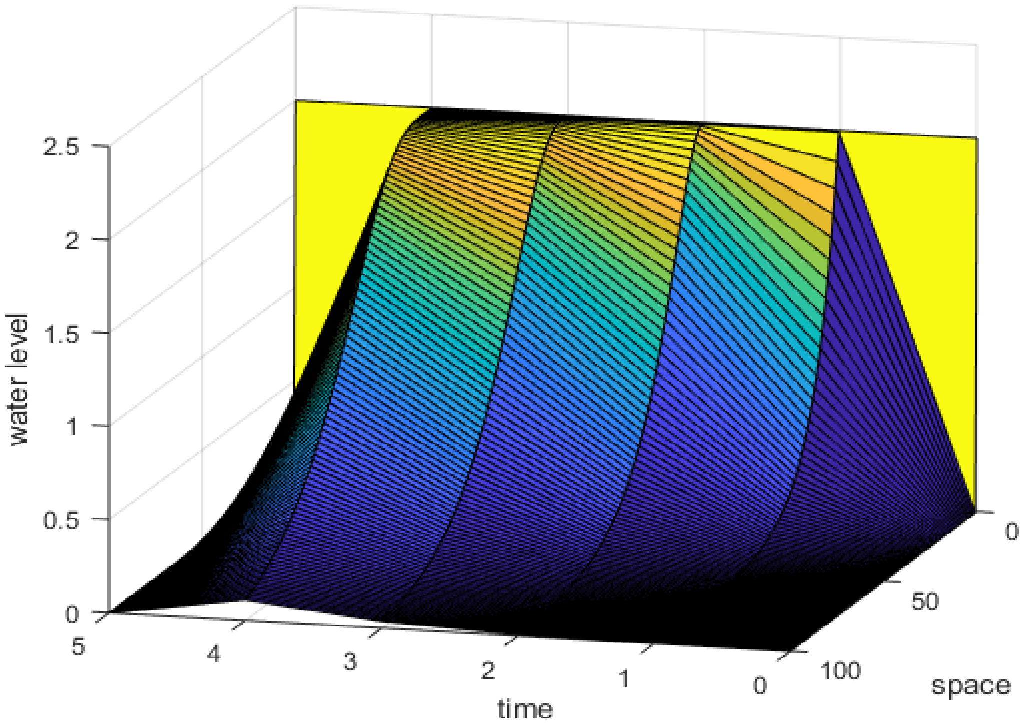

Figure 11: Reduction of water level for delay constant 3, average transmissivity T =405, specific yield =0. 002

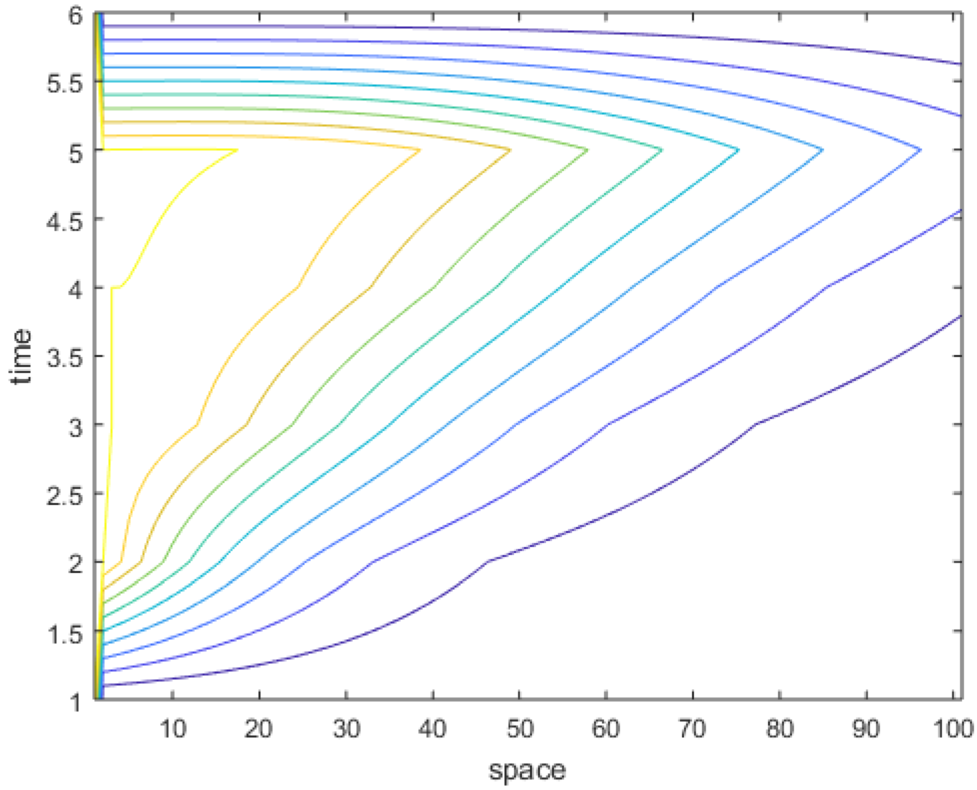

Figure 12: Contour plot solution for delay constant 3, average transmissivity T =505, specific yield =0. 025

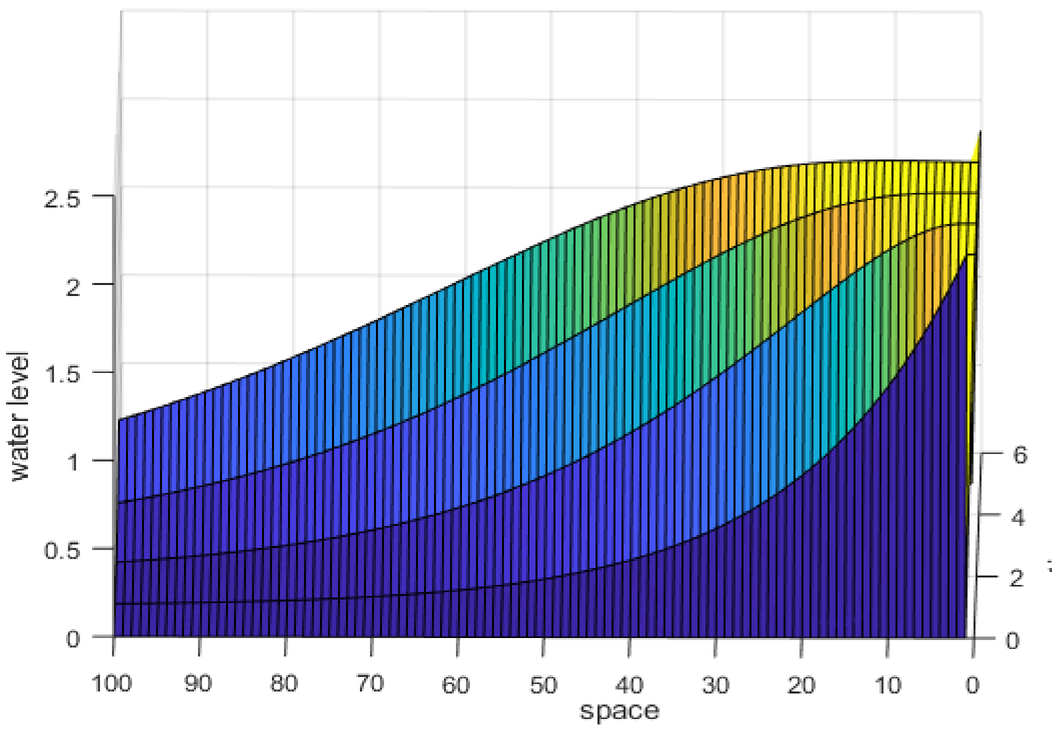

Figure 13: Reduction of water level for delay constant 3, average transmissivity T =505, specific yield =0. 025

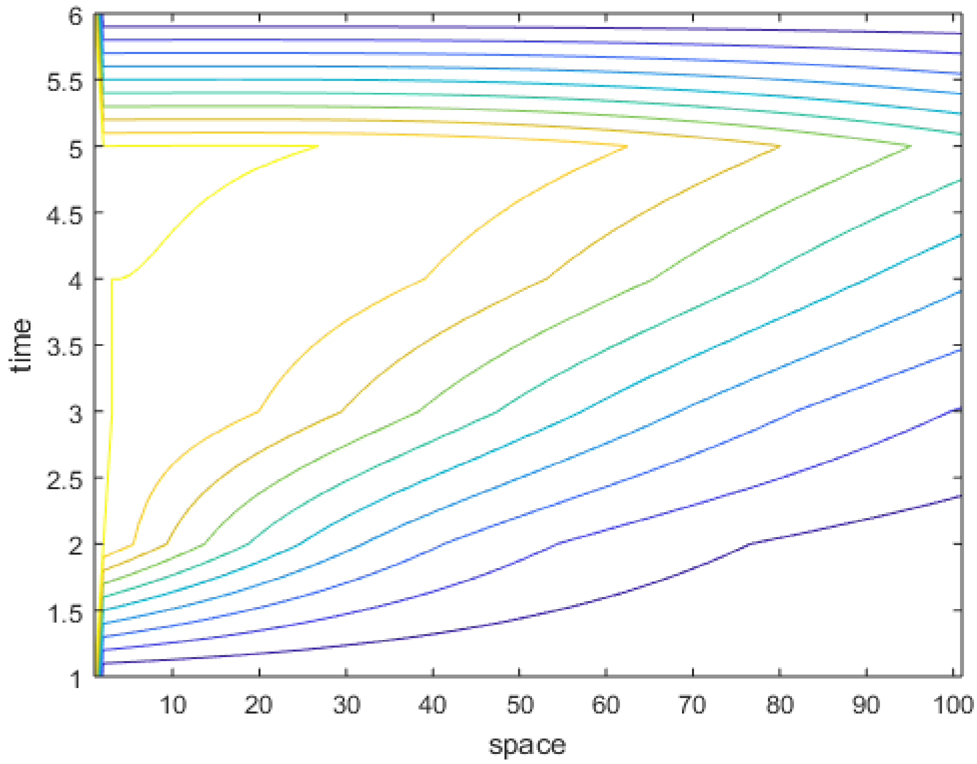

Figure 14: Contour plot solution for delay constant 3, average transmissivity T =555, specific yield =0. 3

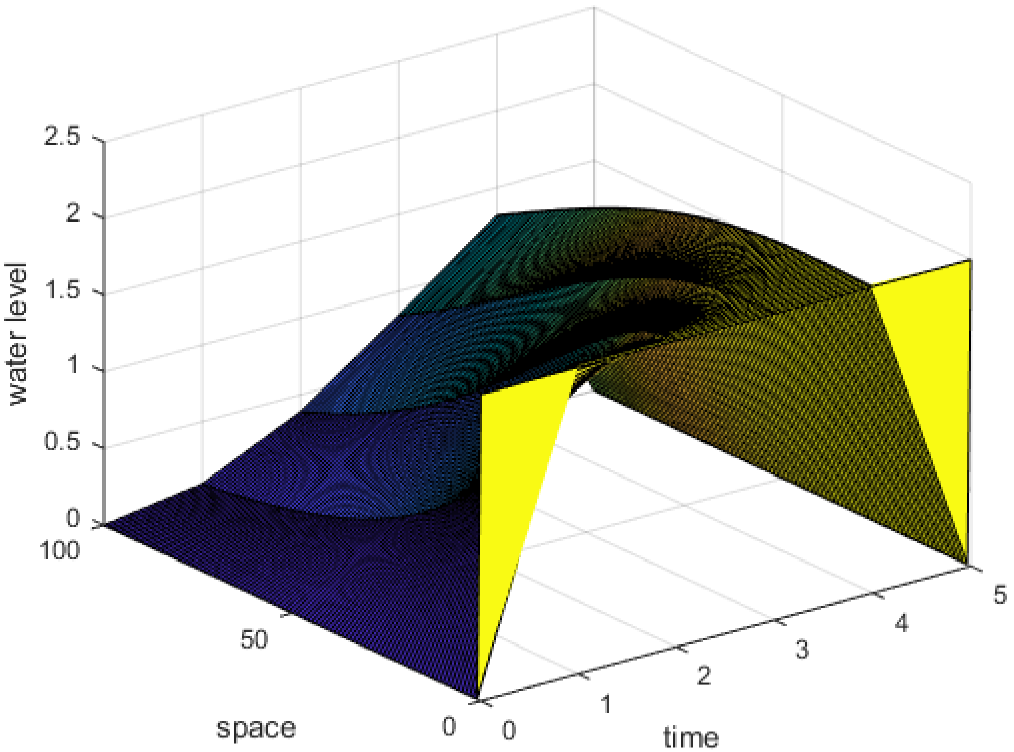

Figure 15: Reduction of water level for delay constant 3, average transmissivity T =555, specific yield =0.3

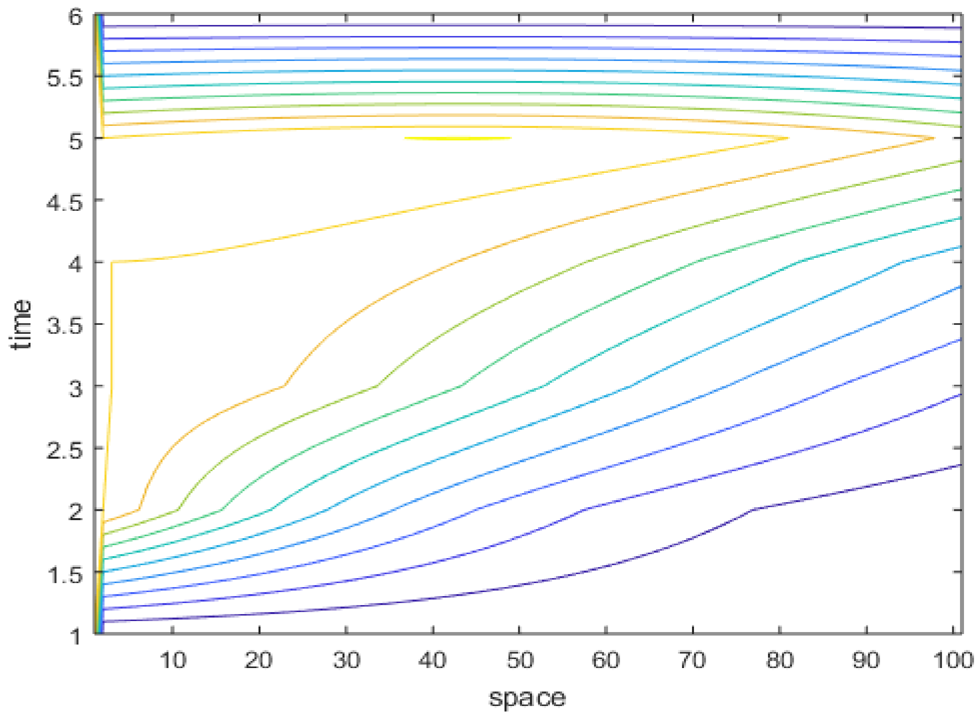

Figure 16: Contour plot solution for delay constant 3, average transmissivity T =600, specific yield =0. 303

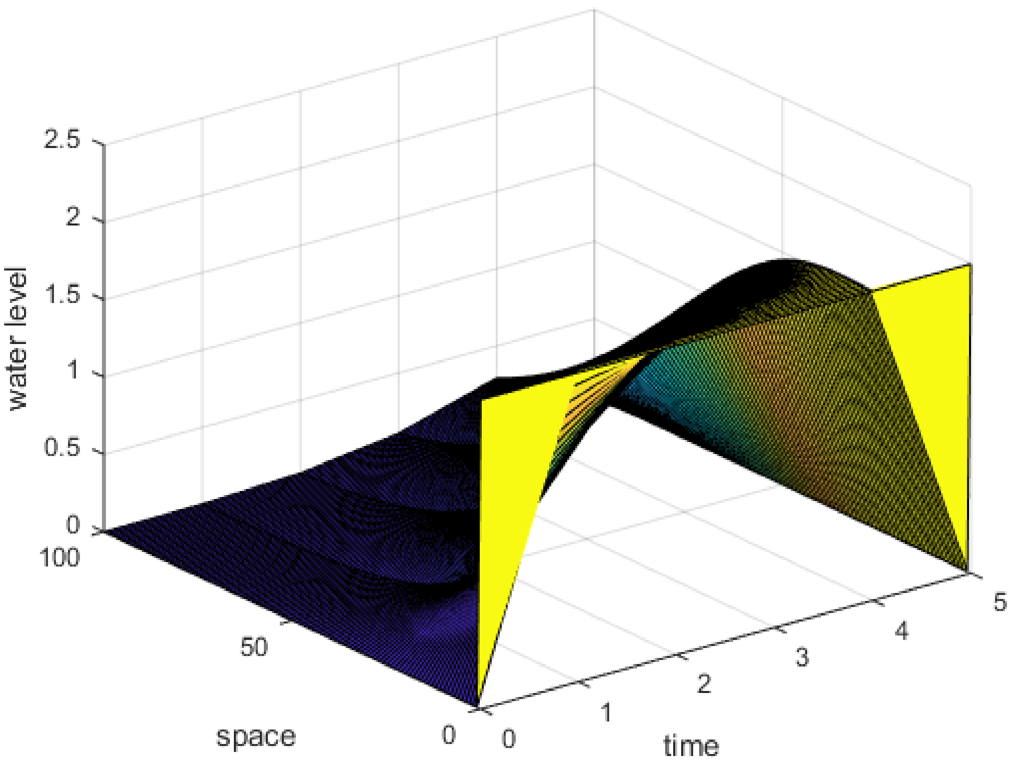

Figure 17: Reduction of water level for delay constant 3, average transmissivity T =600, specific yield =0. 303

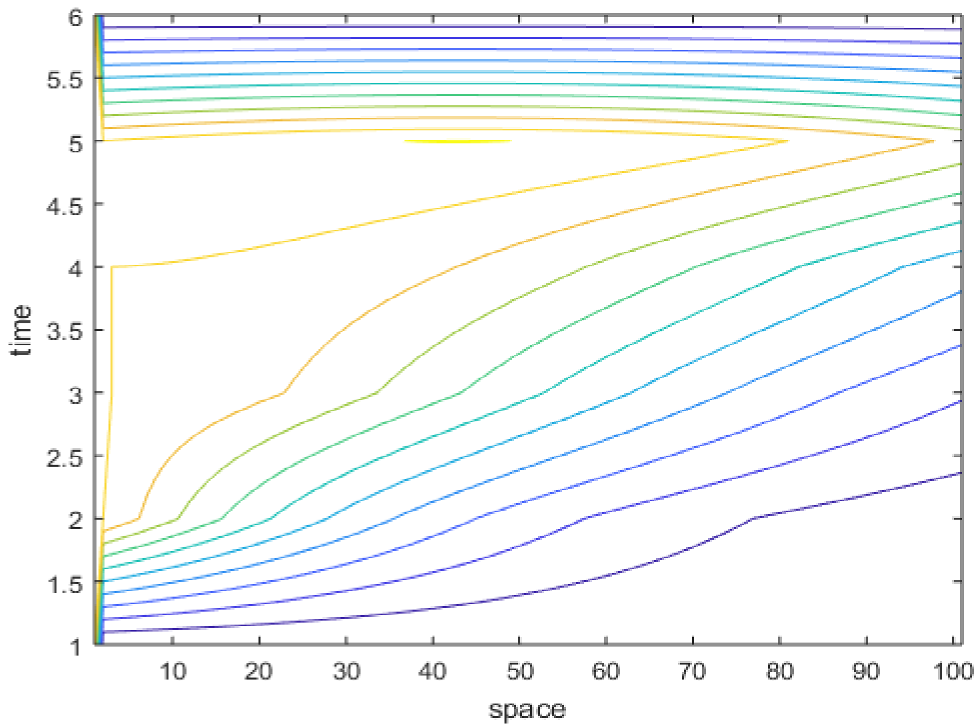

Figure 18: Contour plot solution for delay constant 3, average transmissivity T =650, specific yield =0.304

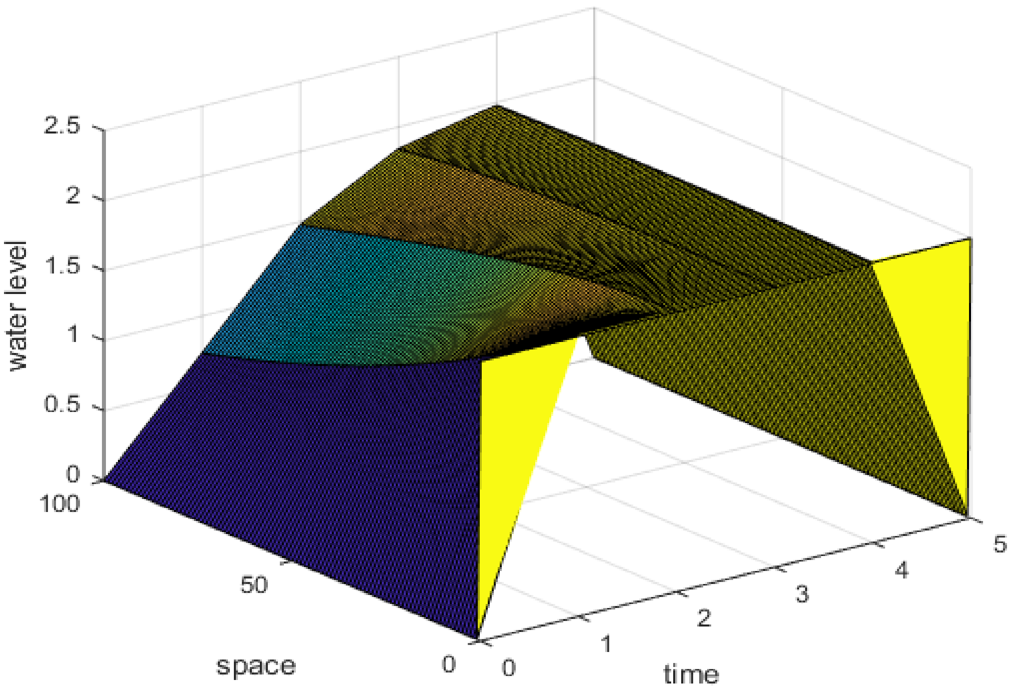

Figure 19: Reduction of water level for delay constant 3, average transmissivity T =650, specific yield =0.304

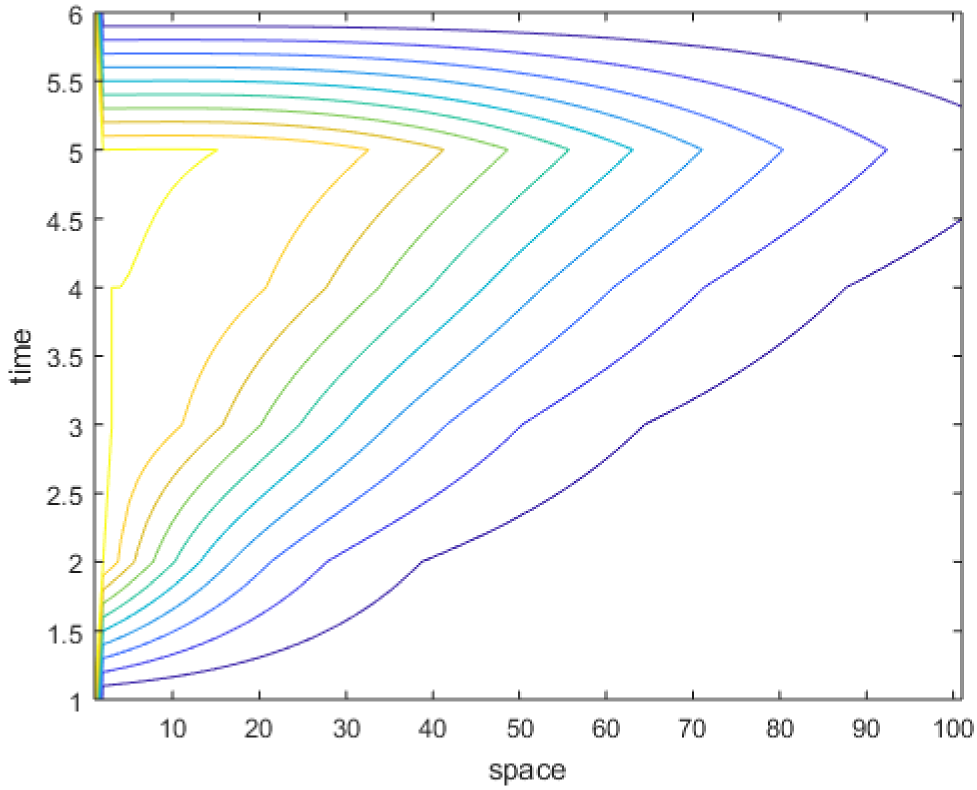

Figure 20: Contour plot solution for delay constant 3, average transmissivity T =700, specific yield =0. 32

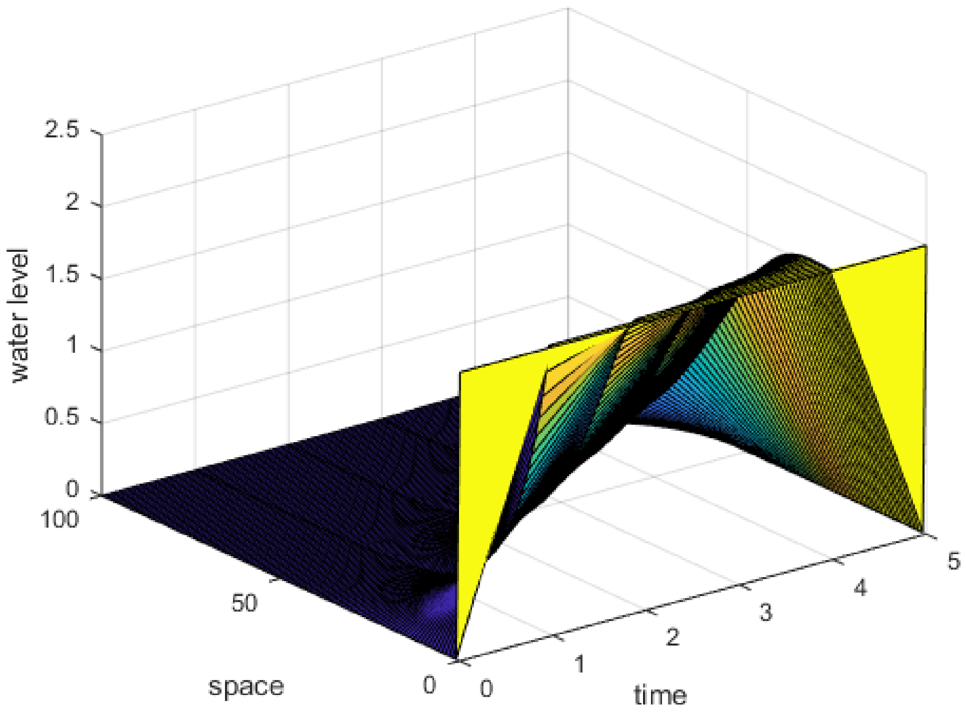

Figure 21: Reduction of water level for delay constant 3, average transmissivity T =700, specific yield =0. 32

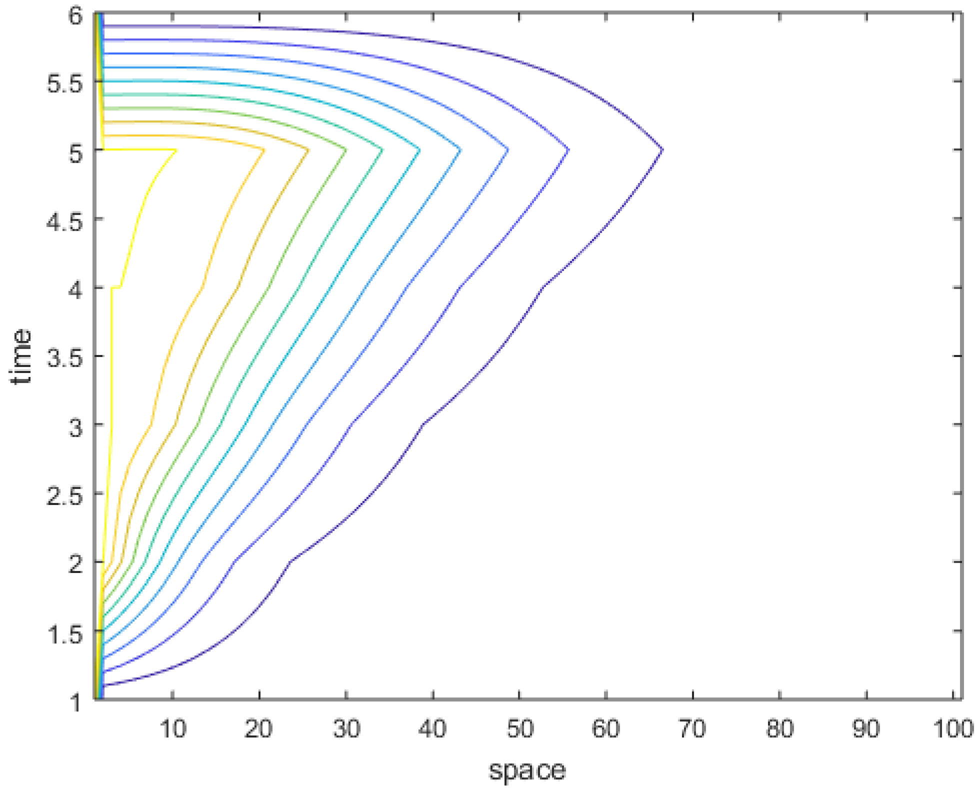

Figure 22: Contour plot solution for delay constant 3, average transmissivity T =800, specific yield =0. 35

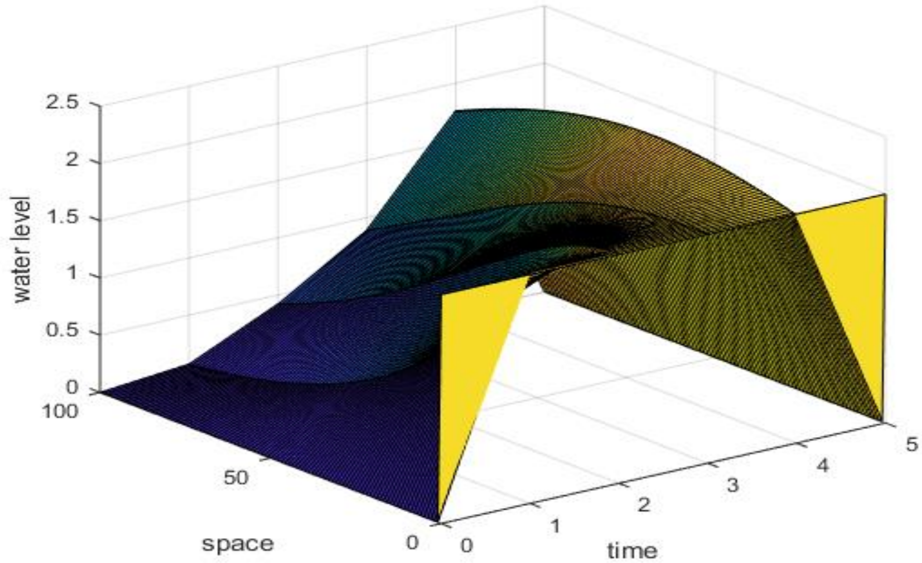

Figure 23: Reduction of water level for delay constant 3, average transmissivity T =800, specific yield =0. 35

7.1 Results and discussions

The above simulations depict that aquifer parameters such as transmissivity, Specific yield and storativity vary with a reduction of water level due to heterogeneities of the geologic nature. The deterministic model which assumes homogeneity falls short in that, natural occurring processes can never be known with certainty. Thus, even if the physics of the system is fairly easy and comprehensible by deterministic equations, it is difficult to fully support the solutions of deterministic models mostly because the input variables, model geometry, initial and boundary conditions and so on are not very well known or, in the ideal case, never known extensively. Stochastic techniques can be considered as a mechanism for combining physics, statistics and uncertainty in a meaningful theoretical context. On the one hand, statistic distributions describe the unknown parameters. On the other hand, the various parameters that describe the problem are related to each other and the (uncertain) model parameters through physical laws (deterministic). The resulting models are partial differential stochastic equations. Returning to the basic groundwater example, recharge (r) and inflow (q) are not very well known. These two variables can therefore be seen as random functions that vary greatly in space and/or time, and also have statistical properties (such as a variance, covariance and mean) that can be inferred from samples. It therefore becomes essential to take into account the heterogeneity that comes with natural occurring processes when modelling.

CONCLUSION

Traditionally, the movement of groundwater was modelled in a deterministic fashion, which assumes that aquifer parameters and boundary conditions are known with certainty. Additionally to the already mentioned uncertainty, it is also assumed that the aquifer's parameters are constant everywhere within the geological formation, which in practice cannot be validated as the subsurface are subjected to heterogeneities. In reality, hydrological events are better described as random phenomena. The aquifer properties, such as, hydraulic conductivity, transmissivity, and storativity will depend on the properties of the soil which is naturally different from one point to another due to the variability of the geology. From already published research works, it was well established that, modelling groundwater flow with constant parameters can only be applicable if the geological formation is homogeneous. However, otherwise, it is preferable to capture some heterogeneities using the concept of stochastic modelling, where a given aquifer parameter is considered to be a distribution. Groundwater flow is therefore more realistically modelled via the stochastic approach. The aim of this dissertation is to distinguish between the deterministic and stochastic model, thus say which is realistically fit to model the flow of groundwater in the unconfined aquifer system. The main aim of this research was achieved through the analysis performed from the two numerical schemes. Although some researchers still use the deterministic approach to model the flow of groundwater, results have proven that the stochastic approach is realistically fit to model the flow of groundwater since it relies wholly on uncertainty which is expected to happen in nature due to heterogeneity of natural occurring geological processes. This research enabled us to see how the assumption of homogeneity on natural processes can lead to incorrect interpretation. The numerical simulations showed graphical representations of the flow of groundwater and how varying aquifer parameters as well as keeping them constant affect the simulations which is appropriate for the modelling of regional groundwater models.

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APPENDIX

```
Numerical coding from MATLAB Software
Lmax = 5;
Tmax = 100;
maxt = 100;
h = Tmax/maxt;
n_spaces = 5;
dx = (Lmax/n_spaces);

%Parameters to be used
alpha1 = 4;
Sc = 0.001;
Sy = 0.091;
B = 1;
T = 800;

%Initial and boundaries conditions
for i = 1:(n_spaces+1)
    x(i) = (i-1)*dx;
    H(i,1) = 2;
end

% matrix vector
for n=1:maxt+1
    t(n) = (n-1)*h;
end

a1 = 1/(alpha1*(dx^2));
a2 = 1/(alpha1*dx);
a3 = (alpha1*Sy)/(T*dx);

alpha = 1;
Ma = 1;

for n=0:maxt-1

    for j=2:n_spaces
        dh = a1*(H(j-1,n+1)-2*H(j,n+1)+H(j+1,n+1))+a2*(H(j,n+1)-
H(j+1,n+1))+a3*(H(j,n+1)-H(j+1,n+1));
        H(j,n+2) = H(j,n+1) + (((1-alpha)/(Ma)) + ((3*alpha*h)/(2*Ma)))*dh
- (((1-alpha)/(Ma)) + ((alpha*h)/(2*Ma)))*dh;
    end

end

figure
surf(x',t,H')
ylabel('space')
xlabel('time')
zlabel('water level')

figure
contour(H)
xlabel('space')
ylabel('time')
```