2014

Stochastic Approach In Groundwater Modeling: A Case Study Of The Buffalo Creek Watershed

Jenberu Lemu Feyyisa
North Carolina Agricultural and Technical State University

Stochastic Approach in Groundwater Modeling:

A Case Study of the Buffalo Creek Watershed

Jenberu Lemu Feyyisa

North Carolina A&T State University

A thesis submitted to the graduate faculty

in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Department: Civil, Architectural and Environmental Engineering

Major: Environmental Engineering

Major Professor: Dr. Shoou-Yuh Chang

Greensboro, North Carolina

2014

The Graduate School
North Carolina Agricultural and Technical State University
This is to certify that the Master's Thesis of

Jenberu Lemu Feyyisa

has met the thesis requirements of
North Carolina Agricultural and Technical State University

Greensboro, North Carolina
2014

Approved by:

Dr. Shoou-Yuh Chang
Major Professor

Dr. Manoj K. Jha
Committee Member

Dr. Stephanie Luster-Teasley
Committee Member

Dr. Sameer Hamoush
Department Chair

Dr. Sanjiv Sarin
Dean, the Graduate School

Biographical Sketch

Jenberu Lemu Feyyisa graduated with a Bachelor of Science degree in Hydraulics Engineering from Arbaminch Water Technology Institute, Ethiopia in 1992. In 1997, he earned a PGD in Environmental Engineering from Hydraulics Research Institute, Cairo Egypt. In 2012, he enrolled in the master's program in Civil and Environmental Engineering at North Carolina Agricultural and Technical State University. His research under the supervision of Dr. Shoou-Yuh Chang and Dr. Manoj K. Jha focuses on stochastic approach in groundwater modeling, a case study of Buffalo Watershed in Greensboro, North Carolina

Jenberu has worked as study, design and construction supervision engineer on various water resources (water supply, Irrigation, Drainage, watershed development and flood control) project in Ethiopia. He also worked as project officer for an NGO funded by World bank/IMF. He owned and managed a construction company while in Ethiopia. Feyyisa has conducted a study on solid waste management, a case study of Nairobi, Kenya and presented on the International conference in 2013. He also presented parts of his research on a national conference in 2013. He also conducted a study and model one of the impaired waters of Greensboro area. He is a candidate for the Master of Science degree in Civil Engineering.

Dedication

This work is dedicated to my Dad, Lemu Feyyisa, who passed away last August. His support and continual inspiration has rooted a stirring atmosphere for my academic dedication and excellence.

Acknowledgements

I would like to express my sincere gratitude and appreciation to my advisor, Dr. Shoou-Yuh Chang, and co-advisor Dr. Manoj K. Jha for their insightful suggestions and professional guidance throughout the course of this study. I would also like to thank other member of my thesis committee, Dr. Stephanie Luster-Teasley for her review and invaluable comments on the thesis. Furthermore, I would like to extend special thanks to my wife Meseret Senbeta and my children (Kena and Ifaa) for their support and encouragement which has made this endeavor a possibility.

This work was sponsored by the Department of Energy Samuel Massie Chair of Excellence Program under Grant No. DE-NA0000718. The views and conclusions contained herein are those of the writers and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the funding agency.

Table of Contents

List of Figures

List of Tables

Abstract

Simulation and prediction of groundwater flow and solute (contaminant) transport highly depends upon aquifer parameters and their spatial distribution. Since this variability in space is in fact random, solutions for groundwater flow and contaminants transport are better defined through a statistical approach.

This study acknowledges and considers spatial variability of horizontal hydraulic conductivity values and compares calibrated steady-state condition groundwater flow both in deterministic and stochastic approach using MODFLOW model. Based upon the discretized model, for each model run 10, 495 different horizontal hydraulic conductivity values (set) were generated using Kriging statistical distribution method and results of groundwater depth was compared with measured depth, R^2 value equal to 0.7471. Seven of the eight (87 %) sets of hydraulic conductivity values ranging from 10^{-3} m/second to 10^{-7} m/second generated less error than the deterministic approach. Similarly, using the calibrated parameter, contaminant plume path has also been defined using MT3D model, with five of the eight (62 %) sets of spatially varied hydraulic conductivity values generating less error than the deterministic value for solute mass balance. Potential groundwater paths were also determined and indicated using velocity vectors calculated by MODPATH model. Moreover, contaminant plume propagation in flat slope regions of the watershed showed little advance towards the predefined exits. Rather, higher concentration contours were observed in a limited area, indicating potentially polluted regions of the watershed in shallow aquifer zones that include South Buffalo wetland. Out of the total annual base flow, about 3 %, with expected rise during dry seasons, is contributed by impaired streams through groundwater-stream flow exchange.

Key words: Groundwater, MODFLOW, Contaminant, Buffalo watershed, MT3D, ArcGIS, Stochastic, Deterministic

CHAPTER 1

Introduction

1.1 Background

Groundwater is not only a valuable source for drinking water; it is also important for agriculture and industries. Being filtered through soil grains it is usually clean and fresh. Today, this valuable natural resource is threatened because of human activities, sometimes even without realizing how they are affecting its quantity and quality.

Human activities expanded in cities, agricultural lands and large settlements. The United States EPA (1991) categorized typical sources of potential groundwater contamination by land use category as: Agriculture, Commercial, Industrial, Residential and others. Urbanization can dramatically alter the hydrological cycle and water quality standards since most of these sources are results of it. Groundwater contamination by metallic elements and organics is nearly always the result of human activity and causes hazards or pose health risks to human. However, the movement of these particles and their effects in the groundwater system cannot be traced and detected easily due to the complex nature of media of transport (aquifer system). Timeframes between an original pollution event, percolation through the unsaturated zone, transport in groundwater, and eventual base flow discharge to a receiving river may be years to decades later and depend upon the pathways and distances involved, groundwater velocities and capacity for natural attenuation of a pollutant in the subsurface (Rivett el at. 2011).

In many of the previous water quality studies and environmental impact assessments, too much attention was given to surface water sources because either they relegate its potential impact on the environment or difficult to understand and solve analytically. This hinders the importance and long term effects of groundwater contamination. In some instances, the study of surface water quality is also assumed to include groundwater quality too. Typically, groundwater inputs are not included in the estimate of waste load, because of these, resources required to study and mitigation measures are skewed towards surface water sources (Winter et al., 1998), rehabilitation of the subsurface environments is seldom considered as a goal (Boulton, 2007). In some cases, water-quality standards and criteria cannot be met without reducing contaminant loads from groundwater discharges to streams (Winter et al., 1998). They also added pollution of surface water can cause degradation of groundwater and conversely pollution of groundwater degrades surface water. Bergstrom et al., (2007) discussed that the full range of environmental and economic services of groundwater needs to be accounted for in policy decisions.

Surface water quality alleviation measures such as riparian wetland have shown significant changes through biochemical processes. Simultaneously, it also facilitates flux of particles (contaminants) into groundwater. A simulation in which the floodplain sediments of low saturated hydraulic conductivity at the re-meandered site were replaced with sandy gravels increased downwelling stream water by 10 times (Kasahara et al., 2008). Such activities may also lead to deterioration of groundwater quality in shallow aquifer regions due to rapid exchanging behavior of surface water and groundwater. Much of groundwater contamination in the United States is in the shallow aquifers that are directly connected to surface water (Winter et al., 1998). Greater knowledge of the water-quality functions of riparian zones and the pathways of exchange between shallow groundwater and surface-water bodies is necessary to evaluate the effects of riparian zones on water quality (Winter et al., 1998).

To begin addressing pollution prevention or remediation, we must understand how groundwater and surface waters interrelate. Groundwater and surface water are interconnected and can be fully understood and intelligently managed if only when the fact is acknowledged (EPA). As a function of groundwater in the hydrologic cycle and ecosystem are better understood, funding decisions to prevent adverse effects to the resources will more fully recognize groundwater's role. The need to understand groundwater system and its interaction with surface waters and stressors (contaminants) is one of the areas where recent studies give attention due to its paramount need.

The amount of ground water available from the regolith-fractured crystalline rock aquifer system in Guilford county, North Carolina, is largely unknown (Daniel et al., 1989). They also underscore, non-recognition of these services imputes a lower value for the groundwater resources in establishing policies. Planners and managers benefit from additional knowledge of ground water resources.

1.2 Regional Assessments and Trend

Agriculture and industry are the main sources of pesticide and heavy metals contamination of surfaces waters in North Carolina (Kenneth, 1993). Pfaender et al. (1977) examined the Cape Fear River basin for metals and found lead values exceeding the maximum level recommended by EPA for public water supply at two sampling sites. In a similar year, trace amounts of chromium, cadmium and copper found near industrial and municipal sources near Greensboro and Burlington, North Carolina. Davenport (1989) examined water samples collected from the Reedy Fork and Buffalo Creek basins in Greensboro and found a significant difference in concentration of calcium and magnesium in samples taken from urban and rural areas. Davenport (1989) also reported levels of iron, copper, zinc, arsenic, phosphorous, manganese and cyanide and mercury in excess of state and/or federal water quality standards. The segments of North and South Buffalo Creek in the Greensboro area constitute one of the worst water quality problems in North Carolina. Conductivity continues to increase in these streams (medium values are greater than 550 µmhos/cm), nutrient values are high, and there are chronically high levels of dissolved copper, zinc and cadmium (NCDNRE, 1999). The City of Greensboro (2010) discussed that (our laboratory must conduct over 10,500 test per year. Any one of these tests may result in a value that causes us to violate the limits of the NPDES permit. There are some limits such as cyanide, fluoride, selenium and cadmium over which the operators of the treatment plant have no control other than through regulating what industries and households can discharge to the sewer). EPA in its consecutive reporting years since 1970's, categorized Buffalo Creek Water as threatened and/or impaired water. Just as groundwater moves slowly so does contaminants in groundwater. Because of this, the current amounts of contaminant concentrations are expected to increase significantly once groundwater plumes discharge into streams.

1.3 Problem Statement and Motivation

Once groundwater is contaminated, it is difficult and expensive to clean. Moreover, this is irreversible in areas where the quality is deteriorated. Modeling of groundwater flow and investigating fate of contaminants enable us to understand the present and future trend of groundwater quality and quantity. Buffalo Creek is one of the streams in the piedmont region of Guilford County, North Carolina categorized by Environmental Protection Agency (EPA) as impaired waters of the region from its designated purpose (aquatic life propagation and survival). The causes of impairment are metals (Cooper, Zinc, and Ammonia un-ionized) and Biological Integrity Benthos (EPA, 2008 and 2010). Changes in the natural interaction of groundwater and surface water caused by human activities can potentially have a significant effect on the environment. Similarly, due to their geographical location the streams water quality of Cape Fear River waters can affect downstream water bodies. All water users downstream of Guilford County are directly affected by stormwater that drains from the Greensboro metropolitan area (the City of Greensboro, 2011).

Terziotti et al., (1994) indicated that a significant population size of Guilford County depends on the shallow groundwater source of the watershed as their primary source of water supply for their household consumption. Approximately 30 percent of the water used in Guilford County, North Carolina, is from groundwater sources. Moreover, all rural supplies are from groundwater; approximately 65,000 residents used groundwater for their domestic water supplies in 1990. The number of residents depending upon groundwater for potable supplies has doubled in the last 15 years and will continue to increase with population growth in the county (NCDWR and Department of Public Health, 2007). Reports indicate that surface water quality is getting worse since monitoring began. Regarding groundwater quality no detailed report is obtained until this report is compiled. Few studies based upon data collected from private wells by North Carolina Department of Environment and Natural Resources (NCDENR) indicated groundwater contamination counts resulted from storage tanks. In all the cases exact location of these wells, frequency of testing, information weather the well is active monitoring or not was not mentioned. Through our personal contact, the City of Greensboro affirmed that there is no groundwater quality monitoring well throughout the County that monitored by their division.

1.4 Literature Review

Rahmawati et al., (2013) studied salt intrusion in coastal and lowland areas using PMWIN MODFLOW, MT3D, and ArcGIS. They highlighted the salt water intrusion from 1995 until 2108 based on well log measurement and MODFLOW numerical modeling. Groundwater model in study area was simulated for advective transport and hydrodynamic dispersion (mechanical dispersion and mechanical diffusion) using solute transport model MT3D. They presented spatial and temporal salt intrusion in the past, present and future. Their results showed that, the movement of saline groundwater from coastline to landward years by years from 2018, 2028, 2048, 2068, 2088 and 2108 following the high hydraulic conductivity area. They also find out that salt intrusion was also driven by future sea level rise which result to the increase of the fresh waterfront forward move.

Simulation of groundwater flow using MODFLOW and transport of dissolved solids in terms of Electrical Conductivity (EC) using MT3D models were conducted by Abu-EL Sha'r et al. (2007) in the watershed area that consists of 600 water wells. The models were used as a management tool for the well field that extracts water in excess of the aquifer safe yield for domestic and agriculture demands. This led to a sharp drop in water table and drying out of springs that resulted in increase of salinity in most parts of the basin. For the year 2005 through 2020, five different scenarios; maintaining the current pumping rate, reducing the current pumping rate by half, increasing the pumping rate by half, reducing public wells pump by half and maintain other wells with the current rate and reducing agriculture wells pumping by half keeping others rate with the existing rate were proposed. They found that scenarios first and fourth had a similar effect on drawdown. Similarly, second and fifth scenarios had a similar effect and also provide lowest drawdown. The third scenario provided worst drawdown. After adjusting parameters that include EC and boundary and advective parameters, the run MT3D model and found that the effect of scenarios on the value EC is less profound than the effect of drawdown.

Kasahara et al., (2008) conducted study of the relative effect of individual elements of lowland stream restoration projects on stream–subsurface water exchange has been conducted. The study sites were modeled to simulate water exchange between the stream and streambed, constructed gravel bar and meander bends, using a 3D finite difference model, MODFLOW in a graphical user interface. A set of cells along the constructed features was selected in MODFLOW, and the flow budget command was used to calculate these fluxes (volume per unit time per meter stream length). The relative effect of individual elements of restoration projects on stream–subsurface water exchange was studied by identifying elements that were most effective in increasing downwelling stream water (DSW) into subsurface environments using groundwater flow modeling. For each MODFLOW simulation, MODPATH was used to simulate the flow path of downwelling stream water (DSW) and mixing of groundwater and stream water in the saturated zone below and adjacent to the stream channel was simulated using MT3D, a solute transport module. Simulations using a homogeneous field of mean hydraulic conductivity that removed heterogeneity showed a large decline in DSW in the four restoration projects studied, suggesting that use of coarse sediments in construction initially increases stream–subsurface water exchange, but the effects may not persist in streams where fine sediments clog streambeds. They also find out that, a simulation in which the floodplain sediments of low saturated hydraulic conductivity at the re-meandered site were replaced with sandy gravels increased DSW by 10 times.

Haro et al. (2011) conducted study on a framework for stochastic optimization of control strategies for groundwater nitrate pollution from agriculture under hydraulic conductivity uncertainty. The main goal is to analyze the influence of uncertainty in the physical parameters of a heterogeneous groundwater diffuse pollution problem on the results of management strategies, and to introduce methods that integrate uncertainty and reliability in order to obtain strategies of spatial allocation of fertilizer use in agriculture.

The aquifer has impermeable boundaries and steady-state flow from top to bottom of the domain. MODFLOW (McDonald and Harbough, 1988), a three dimensional finite difference groundwater flow model, and MT3DMS (Zheng and Wang, 1999), a solute transport model for simulation of advection, dispersion and chemical reactions were used. The transport solution techniques include the standard finite difference method, the particle-tracking based Eulerian–Lagrangian methods, and the higher-order finite-volume TVD method. A pollutant concentration response matrix was generated for each *K* realization. The domain was divided into square cells of 500 × 500 m, with a grid made up of 58 rows and 40 columns. A confined aquifer has been modeled with a saturated thickness of 10 m, effective porosity of 0.2, and longitudinal dispersivity of 10 m. The natural annual recharge is 500 m^3/ha. There are 70 stress periods, each of one-year duration (365 days). Deterministic and stochastic distributed hydraulic conductivity values were compared to evaluate the reliability of optimal fertilizer application for an aquifer with a pre-assumed heterogeneous hydraulic conductivity field. Once they generated different conductivity fields, pollutant concentration responses from unit recharge rates at the sources were simulated.

Their results show a high probability of not meeting the groundwater quality standards when deriving a policy from just a deterministic analysis. They also commented; to increase the reliability several realizations can be optimized at the same time. By using a mixed-integer stochastic formulation, the desired reliability level of the strategy can be fixed in advance.

1.5 Objective of the Study

Field and laboratory test results of hydraulic conductivity indicates variation in the order of kilometers. These variations, in fact, can be encountered within meters and centimeters distance both vertically and horizontally. Hydraulic conductivity varies by up to five orders of magnitude over a distance of less than a meter vertically and about 100 meters horizontally (Gego et al., 2011). This variability, in a space, is, in fact, random. The highly spatial organization of conductivity, most specifically the continuity and connectivity of the highly conductive paths is of extreme importance for groundwater flow and contaminant transport simulation.

Consequently, if the general groundwater flow equation represents randomly distributed parameters then, solution of groundwater flow and contaminants transport are defined through statistical method. For this reason, the use of groundwater flow and transport simulation model in a deterministic frame model may not be adequate. Haro et al. (2011), in their study on the framework for stochastic and deterministic optimization of control strategies for groundwater nitrate pollution from agriculture under hydraulic conductivity, found that, high probability of not meeting the groundwater quality standards when deriving a policy from just a deterministic analysis.

The overall all goal of this study was to examine the flow path and characteristic of contaminant transport in the piedmont region of North Carolina. North and South Buffalo sub-watershed of 229.2 km^2 was selected for model development and analysis. The specific objectives are;

1) Develop a groundwater flow and contaminant transport model using PMWIN

2) Calibrate MODFLOW for groundwater flow movement

3) Compare deterministic and stochastic approach for modeling groundwater flow under steady state condition

4) Determine fate and transport of contaminants including plume paths

The specific objectives of the study was then setting up of numerical groundwater model that describes the aquifer behavior including hydraulic head, and then predict fate and pattern of contaminants. Generally, this study can provide necessary tools and understanding of groundwater flow and fate of contaminants within the watershed. Environmentalists and decision makers can get information, on the potential susceptible zones of the watershed against contaminants that can adversely affect the environment. It also helps in highlighting the need for future measures and management alternatives before the poor water quality leads to a point where difficult to reverse.

CHAPTER 2

Site Descriptions

2.1 Location and Climate

The study was conducted on 229.2 square kilometers of Buffalo Creek (USGS hydrological unit 03030002) watershed in Guilford County North Carolina. Located in the Upper Cape Fear River basin, the watershed is made up of two 12 HUC watersheds (North Buffalo and South Buffalo) that include most parts of Greensboro city. Generally, the river basin is characterized by a shallow unconfined regolith aquifer. The geospatial area is bounded between 79^0 38'47"- 80^0 W and 36^0 – 36^0 09' 11" N. Surface elevation varies from 256 m (amsl) at upstream water divide line to 202 m (amsl) at its downstream exit. There are nine 12 digit HUC watersheds border Buffalo watershed. Reedy Fork (Lake Brandt, Lake Townsend and Smith Branch); Upper Deep River (High Point Lake, Bull Run and Hickory); Lower Deep; Little Alamance (Upper and Lower little Alamance) from North, southwest, south, and southeast respectively, Figure 1. The topography of the area consists of low rounded hill and long, northeast-southwest trending ridges with up to few hundred feet of local relief (Daniel et al., 1998).

The Climate of Guilford County is typed as humid-subtropical with mean minimum January temperatures range from 31 to 33 ^{0} F whereas mean maximum July temperature range from 87 to 89 ^{0} F. Annual precipitation varies across the county from 43 to 48 inches (Kopec and Clay, 1975). The lowest rainfall occurs in the southern and southwestern parts of the county; the highest rainfall occurs in the southern and southeastern parts of the county (HERA Team, 2007).

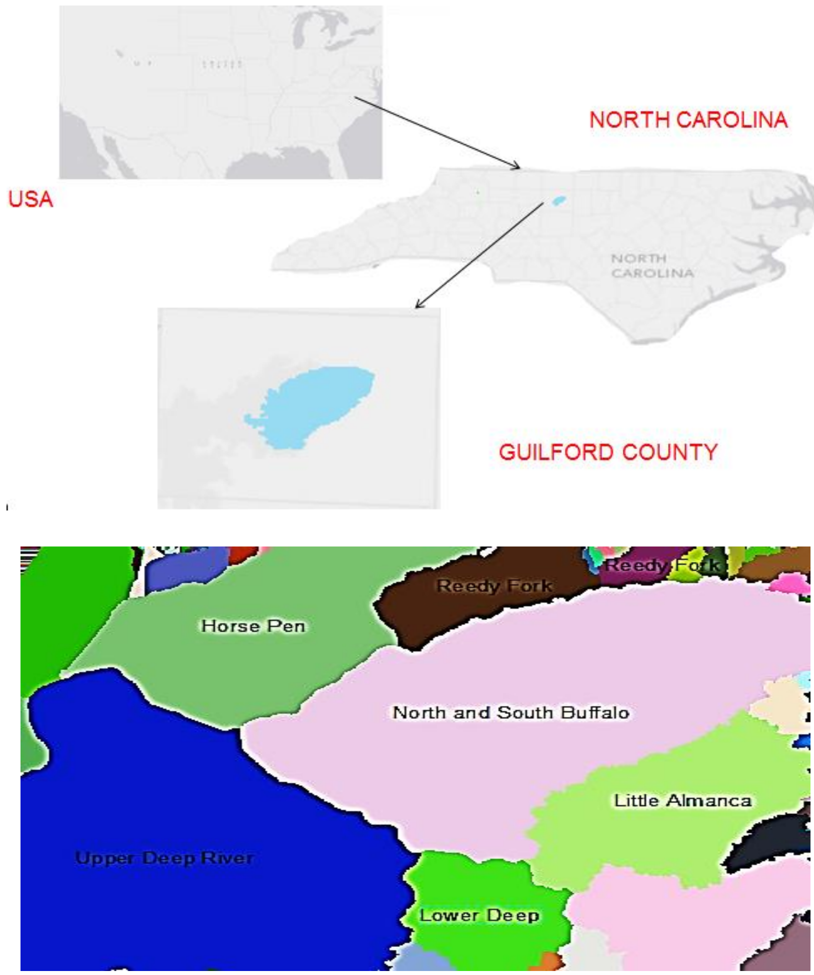


Figure 1 Location map of Buffalo and neighbouring watersheds

2.2 Subsurface Materials and Types

Geologically, Guilford County lies within the Charlotte Slate Belt. Metamorphic and Igneous crystalline rocks are mantled by varying thickness of regolith (HERA Team, 2007). Daniel et al., (1998), in their Idealized Sketch of the groundwater system, categorized the regolith aquifer geological setting of the Guilford County as: (1) the unsaturated zone in the regolith, which contains generally, the organic layer of the surface soil, (2) the saturated zone in the regolith, (3) the lower regolith which contains the transition zone between saprolite and bedrock and, (4) the fractured crystalline bedrock system. Regolith layers consist of loose, heterogeneous material that covers the underlying bedrock. This includes dust, soil, broken rock and also other materials. The transition as the name indicates is a layer that extends from the saturated regolith to the bedrock. It consists of particles ranging in size from silt and clays to large boulders of un-weathered bedrocks. Daniel et al., (1989) discussed that, the transition zone unconsolidated materials grade into bedrock. From their carefully augured wells in three places within the piedmont region, they also indicated that the transition layer is averaged to only 15 feet thick from the estimated combined thickness of 97 feet that covers 90 percent of the total cased wells depth in the piedmont. This depth also reduced to less than 10 feet in some places. The average estimated depth of regolith is also reported to be 52 feet.

The consolidated and semi-consolidated texture type of regolith characterizes it as porous media in the groundwater flow system. Because of its porosity, the regolith provides the bulk of the water storage within the piedmont groundwater system (Heath, 1980, adapted from (Daniel et al., 1989). From the idealized sketch, the bulk of groundwater storage is available in the saturated regolith aquifer. The piped connection system in the bedrock indicates that storage from this layer is found along the fractured lines with porosity varying from ten at the interface of the transition down to zero with depth. These fractures serve as intricate, interconnected network of pipeline that transmits water to springs, wetlands, streams or wells (Daniel et al., 1989). They also added that the bedrock, on the other hand, does not have any significant inter-granular porosity. It contains water, instead, in sheet like openings formed along fractures in the otherwise solid rock. This indicates that the storage within the bedrock is very insignificant compared with the upper reservoir, the regolith.

One of the key parameters in describing groundwater flow and solute transport in aquifers is the saturated hydraulic conductivity (K). For various purposes, in-situ aquifer hydraulic conductivity tests were conducted by many researchers and consultant firms within the watershed. In an effort for construction license permit of White Street Landfill site, the city of Greensboro hired different consultants to conduct soil hydraulic conductivity through augured wells. The data from these tests yielded hydraulic conductivity values ranging from 0.042 feet/day in II-5 to 0.380 feet/day in II-3, 0.221 feet/second in II-6 and 2.353 feet/second in II-8 (BPA Inc., 1996). For those samples that are representative of the saprolite just above the water table (SB-46, SB-47 and SB-50), undisturbed permeability ranged from 1.0 x 10^{-6} to 2.7 x 10^{-7} cm/second and the remolded ranging from 3.3 to 3.9 x 10^{-7} cm/second (HDR Inc., 1997). Price et al. (2010) found that the average field K_{sat} of the forest soils was approximately seven times greater than the lawn and pasture soils, which were highly similar (forest = 77 mm h^{-1}, lawn = 11 mm h^{-1}, pasture = 12 mm h^{-1}). Based upon these test results, average horizontal hydraulic conductivity value was estimated to be between 10^{-5} to 10^{-6} m/second.

Porosity indicates the total volume of space in the rock. Because part of the fluid in the pore space is immobile or partially immobile due to the attraction of solid surface of the porous matrix by the fluid molecules adjacent to, effective porosity is usually less than porosity value. PMWIN transport models (PMPATH, MT3D) use effective porosity to calculate the average velocity of flow in the aquifer. The porosity of regolith is typically about 35 to 55 percent in the soil and saprolite but decreases with depth (Stewart et al., 1962), bedrock porosity is 1 to 10 percent but for North Carolina Piedmont is 1 to 3 percent, (Freeze and Cherry, 1979).

2.3 Evapotranspiration

Based on the data presented in National Oceanic and Atmospheric Administration NOAA (Farnsworth et al., 1982), annual pan evapotranspiration loss is estimated to 51.72 inch. Criddle, (1958); Schulz, (1973) estimated potential evapotranspiration rate to 40 inches/year in central piedmont region. From 40 years record of weather data in the central and eastern North Carolina, Winner and Simmons, (1977); Daniel, (1981); Daniel and Sharpless, (1983) averaged actual evapotranspiration value between 21 to 30 inches/year. They also estimated excess evapotranspiration as 13 inches/year while setting up the actual evapotranspiration to 27 inch/

year. Annual volume of water lost through evapotranspiration is calculated by multiplying the annual depth to the total drainage area. This eventually helps in determining the net recharge rate to the aquifer via simple water balance equation.

2.4 Regional and Local Groundwater Table

In two transects across south Buffalo Creek, Matthews, (2002) constructed ten wells to determine the water table regimes and conclude that fluctuation of groundwater is estimated between 0.5 to 3 m from the ground surface. Gibsonville observation well is located at about 10.5 km (GIS measurement) southeast of Buffalo watershed at coordinate's latitude 36^0 5' 17.7" N and longitude 79^0 32' 52.50" W. Elevation of the ground surface at well is 197.5 m (amsl). From the available groundwater level data (2000-2012), annual average values were downloaded from USGS/NCWRD web site. Box plot was prepared to depicting graphically the observed water level data, *Figure 2*. The median value was approximated to 189.8 m (amsl). The first and third quartiles also approximated to 188.8 m and 190.2 m amsl respectively.

Yow 2 observations well is located at about 5.3 km South of Buffalo Watershed boundary. It is located at latitude 35^0 57' 30.19" N and longitude 79^0 50' 19.12" W in Deep river watershed at ground surface elevation of 246.88 m (amsl). Annual average water level data is available from 2000 to 2004. Similarly from the box plot annual average groundwater level was approximated to 245.5 m (amsl).

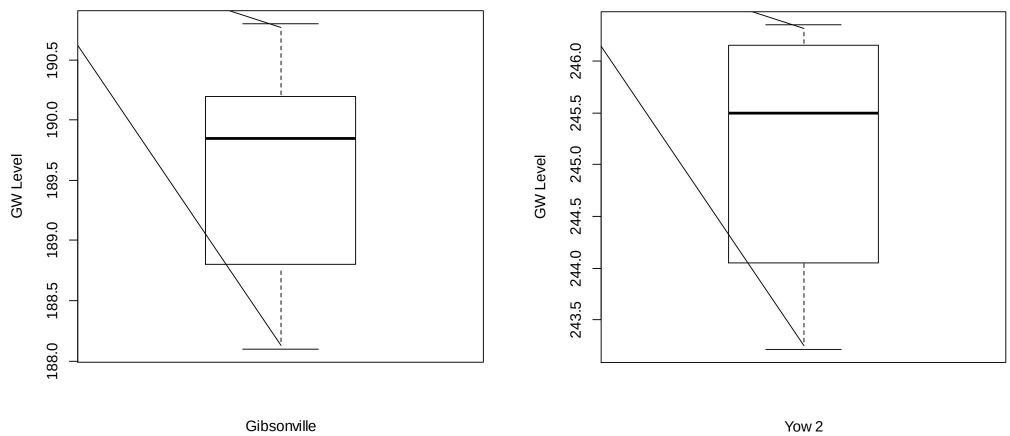


Figure 2 Box plot, annual groundwater depth fluctuations statistics for Gibsonville and Yow2 observation wells

For Gibsonville, the average maximum and minimum data were evaluated, and its average annual groundwater depth was estimated to be 189.5731 m (amsl). Daniel et al. (1998) estimated groundwater fluctuation between 4 to 12 feet in the piedmont region. The variation of aquifer depth in Orange County is between 42–46 feet below ground surface, (Cobel at el. 1989).

2.5 Groundwater Flow and Sources

Geographically, Upper Cape Fear River Basin is located on the headwaters of Cape Fear river basin. The sub-water shed divides Cape Fear river basin from other two main watersheds of the state, Roanoke and Yadkin. The upland surface of the basin slopes generally, towards the east or southeast and is characterized by gently rolling hills and elongated ridges (Floyd et al., 1974). Groundwater flow exchange among these main basins is not clear. While, from a geographical point of view, it is not easy to conclude groundwater flow exchange among these main basins is not existence, the influence of surface slope on shallow aquifers cannot be underestimated. Floyd (1974), the source of all water in the upper part of Cape Fear River basin is precipitation (about 45 inch per year).

Eighty three years average rainfall data was available in USGS and NOAA web sites. We estimated the average depth of rainfall to 42.332 inches (1075 mm). Gauging station (hydrologic unit code 0209553650), monitored by U.S. Geological Survey is located at 300 feet downstream the confluence of North and South Buffalo Creeks. Discharge measurement data is available since October 2007. The average annual discharge is estimated to 155.42 cubic feet/second (4.401 cubic meters per second).

Sewage is collected from the city of Greensboro and released to Buffalo Creeks via the two main treatment plants; North Buffalo and T.Z. Osborne water reclamation facility. The treatment plants permitted to process about 40 million and 16 million gallons of sewage per day for T.Z. Osborne and North Buffalo respectively. The discharge estimated from the plant is assumed to be nearly equal to the total water supply required/supplied for the City. The daily water supply demand of the city grows from 12 million gallons in 1960 to 33.4 million gallons in the 2013 (the city of Greensboro, 2009). Nearly all the sewage or wastewater that is generated by customers flows by gravity through sewers that range from 6 to 72 inches in diameter (the city of Greensboro, 2011). In similar reporting year the city also indicated that, every day an average of 27 million gallons of sewage generated is also collected, transported and treated. The original sources of this discharge are Lake Brandt, Lake Higgins and Lake Townsend outside of Buffalo Watersheds.

Based on this, out of the total stream flow recorded (section 3.7.2) 27 million gallons per year comes from sewage release; quantity that matches closely with the city's daily water supply demand (neglect loss). Similarly, measured base flow of Buffalo stream includes both groundwater and effluent discharge. It is also imperative that, such a significant amount of measured discharge is not expected from a small drainage area like Buffalo while having rainfall as a single source.

Using simple mass balance equation;

Inflow – Outflow = Change in storage ($I - O = \Delta S$) (1)

Precipitation – (Runoff + Evapotranspiration + Base flow) = Change in Storage (2)

Climate and surficial changes are also assumed insignificant throughout the data period. Beforehand, actual base flow contributed from aquifer need to be separated from combined measured discharge.

Floyd (1974) suggested that, the source of all water in the upper part of Cape Fear River basin is precipitation (about 45 inch per year). This conclusion was derived from the fact that, Upper Cape Fear River basin is head basin, boundary of major watershed divide line. Similarly, Buffalo watershed is one of the sub watersheds located in the headwater regions of the upper Cape Fear basin. This suggests that, groundwater flow exchange from other watersheds of different basins is less likely. Hence, we assumed that, the actual base flow source for this sub watershed is only the percolated part of rainfall over the entire watershed area. But, gauging station measurements include this actual base flow and also sewage released from the treatment plants. Hence component of the measured discharge includes; actual base flow, surface runoff and sewage discharge. Each of these components needs to be separated using hydrography analysis tools.

CHAPTER 3

Methodologies

3.1 General

ArcGIS created by Environmental System Research Institute (ESRI) was used for geographic data creation, management, integration and analysis. Using different toolsets of ArcGIS, raster data sets; surface elevations, stream flow networks, flow directions, flow lengths, basin boundaries are created analyzed and prepared in ASCII format. Depending upon MODFLOW-PMWIN limitations to process data (maximum cell size of 250,000), raster data of DTED resampled multiple times for matching. Scope of the study and model limitations were major factors in setting up the final grid dimensions and numbers. A three-dimensional steady state model MODFLOW (PMWIN) developed by W.H. Chiang and W. Kinzelbach (1991-2001) was constructed to simulate shallow aquifer of groundwater flow. MODFLOW solves ground-water flow equation using the finite difference approximation method. MODFLOW, now days considered being the de facto standard code for aquifer simulation. Based on MODFLOW solution of the flow equation, MODPATH evaluates particle tracking on cell to cell base. Using head distribution solution of MODFLOW, fluid velocity calculated using Darcy's law. PMPATH is especially convenient and commonly used for stochastic groundwater modeling (Larsson et al., 2012). MT3D is Solute transport model with the method of characteristics and Finite difference method. It uses a mixed Eulerian-Lagrangian to the solution of the three-dimensional advection-dispersive –reactive transport equations. The overall process of modeling has been summarized in Figure 4

3.2 ArcGIS

Geographic Information System (GIS) is a system that helps to manage, analyze and display geographic features from the real world map. ArcGIS 10 tools were used to manage and transform spatial distribution of geospatial parameters. First, from a USGS developed earth explorer interface data of Shuttle Radar Topographic Mission (SRTM) 2000, an approximated geospatial area of the watershed (79^0-80^0 W and 35^0-36^0 N) was identified for downloading. SRTM data was organized and processed from raw radar signals spaced at intervals of 1 arc-second (approximately 30 meters). One of the SRTM elevation data package, the Digital Terrain Elevation Data (DTED) has been used for downloading. DTED is the standard mapping format that regularly spaced grid of elevation points and/or cells. These cells contain a matrix of vertical elevation values spaced at a regular horizontal intervals measured in geographic latitude and longitude units. The approximated region of interest was tiled into two subsets.

In ArcGIS interface the two downloaded data tiles were imported as mosaic data and re-tiled as a single data using data management tools. Resampling was employed to set grid dimensions in accordance with PMWIN limitation and the degree of accuracy required for this study, especially for advective dominant transport, MODPATH and MT3D. Cell size of 200 m X 200 m was considered reasonable dimension.

The re-tiled raster data then filled for any sinks to avoid discontinuity of drainage networks. Using the hydrology tools of ArcGIS, then cells with defined drainage and flow direction were developed for major and tributary streams. While establishing the stream network, output cells with high flow accumulation are only used to identify streams. For the resampled size of raster (200 m X 200 m), high flow accumulation is considered for cells receiving flow from more than 100 output cells. That means; cells with flow accumulation receiving from zero output raster are categorized as highs or peaks that also indicate the boundary of the watershed. Consecutively; cells receiving flow from 1 up to 99 numbers are categorized as undefined direction flow cells. The final feature of the stream channel and links are constructed by thresholding the results of the flow accumulated raster, using different GIS conversion tools,

Figure 8a. While delineating the targeted basin, the analysis extent was narrowed and widen from the original coordinate until the outlet of the basin in question was delineated and visible, from which surface elevation data was extracted and compiled in ASCII format, Figure 5.

3.3 Filter Program

Base Flow Filter Program was used to separate the annual average amount of discharge from groundwater. The model separates the base flow from its direct input, stream flow records. This recursive digital filter method described by Nathan and McMahon (1990) was originally used in signal analysis and processing (Lyne and Hollic, 1979). Filtering surface runoff (high frequency signal) from base flow (low frequency signals) is analogous to the filtering of high frequency signals in signal analysis and processing (Arnold J.G et al., 1999). The stream record data passed over the filter three times: forward, backward, and again forward. Each pass will result in less base flow as a percentage of the total flow. Accordingly, the user gets some added flexibility to adjust the separation to more approximate site conditions.

The equation for the filter is;

$$q_t = \beta\, q_{t-1} + (1 + \beta)/2 * (Q_t - Q_{t-1}) \qquad (3)$$

Where q_t is the filtered surface runoff (quick response) at the t time step, Q_t is the original stream flow, and β is the filter parameter. Base flow, b_t is calculated with the equation,

$$b_t = Q_t - q_t \qquad (4)$$

From U.S. Geological Survey daily record of stream discharge data (1998 – 2013) was downloaded and exported to the filter program. The filter program outputs the calculated base flow for the three round runs in addition to the measured input discharge, Figure 10a and 10b. Averaged 15 years daily minimum total discharge is estimated 55 cubic feet per second (1.56 m3/s) out of which actual base flow (groundwater contribution) is assumed to 13.23 cubic feet per second (0.375 m3/sec). Our discharge flow constitutes over 97 % of the stream below our discharge points at the lowest stream flows (the city of Greensboro, 2011). Our estimate, when compared with the city of Greensboro, looks bit higher. However, the city does not provide details of this measurement. Both groundwater and effluent discharge change significantly over months of the year. However, the report does not support its assumption in either of the cases. In our case, groundwater contribution is estimated to 23 % of the flow. Hence, the shallow aquifer discharges 11.9 x 10^6 cubic meters of water to downstream surface waters annually. This also expected to raise the depth of saturated aquifer to about 0.0511 m (2.01 inches) until it emerges as surface water. Annually, estimated mean recharge in South Buffalo Creek Basin is 5.51 inches ((Daniel et al., 1989). Our estimate looks less than one half of the previous investigations. However, plants root extending deep to the shallow aquifer extract significant quantity of groundwater over seasons of the year as transpiration. In our case the annual total evapotranspiration depth (0.6858 m), was already separated from total recharge. Riparian evapotranspiration may consume on average, as much as 21 percent of groundwater recharge before it discharge to streams as base flow (Daniel et al., 1998).

3.4 MODFLOW

Processing MODFLOW in windows (PMWIN) was originally developed for a remediation project of a proposal site in the coastal region of northern Germany several years ago. At the beginning of the work, the code was designed as a pre and post processor for MODFLOW (Chiang et al., 1996). Developed by Chiang and Kinzelbach in 1995, PMWIN is a complete groundwater simulation system in the world. It is a simulation system for modeling groundwater flow with; the modular three-dimensional finite-difference groundwater model developed by the U.S. Geological Survey (McDonald et al., 1988), the particle tracking model PMPATH for windows (Chiang, 1994) or MODPATH (Pollock, 1988,1989,1994), the solute transport model MT3D (Zheng, 1990) and the Parameter Estimation program PEST (Doherty et al., 1994). The window interface includes all the supporting models (MODFLOW, MT3D, MT3DMS, MOC3D, PMPATH for Windows, PEST2000, and UCODE).

MODFLOW is a computer program created by McDonald and Harbaugh in 1984, simulates one, two or three dimensional groundwater flow using a finite difference solution of the model formulation. It is considered as an international standard for simulating and predicting groundwater condition and groundwater/surface water interactions (USGS). Each simulation feature of MODFLOW has been extensively tested. For that, MODFLOW has been accepted in many court cases, in United States as a legitimate approach to analysis of groundwater systems (USGS, 1997). MODFLOW is divided into a serious of components, called packages. At present, PMWIN supports seven additional packages which are integrated into the original MODFLOW. One of these packages is the stream flow-Routing package (STR1). This particular package is designed to account for the amount of flow in streams and to simulate the interaction between surface streams and groundwater (Prudic, 1988).

3.4.1 The governing equation. The partial differential equation for transient three-dimensional groundwater flow in heterogeneous and anisotropic medium, for confined or unconfined aquifer is expressed as;

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t} \qquad (5)$$

Where:

K_{xx}, K_{yy} and K_{zz} are the hydraulic conductivity along the x, y and z coordinate axes parallel to the major axes of hydraulic conductivities;

h is the potentiometric head;

W is the volumetric flux per unit volume representing source;

Ss is the specific storage of the porous medium; and t is time.

The solution of equation (5) requires the use of a numerical method such as finite difference method in which groundwater flow system is divided into grids of cells. Otherwise, it is practically impossible to solve the partial differential equation that describes groundwater flow. The advantage of an analytical solution, when it is possible to apply one, is that it provides an exact solution to the governing equation, and it is relatively simple and efficient to apply. However, obtaining the exact analytical solution to the partial differential equation requires that the properties and boundaries of the flow and transport system be highly and perhaps unrealistically idealized (Konikow, 2011).

3.4.2 Dimensional approach. The governing equation is related to the dimension approach selected by the modeler. In our case a two dimensional approach is used. , since vertical flow, particularly under stead state flow condition is negligible. We also assumed hydraulic conductivity is constant with depth.

3.4.3 Numerical formulation. The groundwater flow equation is solved using the finite difference approximation method. The flow region is considered to be subdivided into blocks in which the medium properties are assumed to be uniform (USGS, Documentation). However to determine the fate of contaminants it is better to consider the natural heterogeneity of the aquifer, particularly variability of hydraulic conductivity. The plan views rectangular discretization results from a grid of mutually perpendicular lines that may be variably spaced. MODFLOW uses the finite difference method and blocks centered approach. This application replaces the continuous system described by equation (5) with the finite set of discrete points in the space and time, such that the partial derivatives are replaced by terms calculated from the head differences calculated at these points. That means for each cell; there is a point called node at which head is calculated. Accordingly the all watershed is divided into blocks of cells having definite size and geospatial locations, Figure 5. A system of simultaneous linear algebraic difference equations results from this process, which is solved for the head at specific points and time that constitute the approximation to the time-varying head distribution.

MODFLOW is designated to simulate groundwater flow system in the aquifers in which (i) saturated flow condition exists, (ii) Darcy's Law applies, (iii) the density of groundwater is constant and (iv) the principal directions of horizontal hydraulic conductivity or transmissivity do not vary within the system. The groundwater flow equation is solved using the finite-difference approximation.

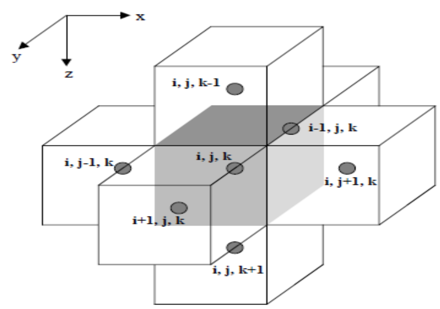


Figure 3 Cell i,j,k and indices for the six adjacent cells (Adopted from McDonald and Harbaugh)

From figure (3), flows are considered positive if they are entering cell otherwise negative. From Darcy's equation, flow in the row direction through the face to a cell from adjacent cell is expressed as;

$$q_{i,j+1/2,k} = KY_{i,j+1/2,k}\Delta x_i \Delta z_k \left(\frac{h_{i,j-1,k} - h_{i,j,k}}{\Delta y_{j-1/2}} \right) \quad (6)$$

The term $KY_{i,j+1/2,k}\Delta x_i\Delta z_k / \Delta y_{j-1/2}$ represents the hydraulic conductance in the row i and layer k between nodes (i,j-1/2,k) and (i,j,k) and h terms represent the hydraulic head at the specified nodes of the cell. The external flow term w of equation (1) represents sources and stresses from outside the aquifer into each cell such as streams, recharge, evapotranspiration wells, can be represented by

$$W_{i,j,k} = \sum_{n=1}^{N} p_{i,j,k\,n}\, h_{i,j,k} + \sum_{n=1}^{N} q_{i,j,k,n} = P_{i,j,k}\, h_{i,j,k} + Q_{i,j,k} \tag{7}$$

$p_{i,j,k\,n}$ and $q_{i,j,k,n}$ are constants that describes the individual external source stresses.

The continuity equation for cell (i,j,k) is expressed as

$$q_{i,j-1/2,k} + q_{i,j+1/2,k} + q_{i-1/2,j,k} + q_{i+1/2,j,k} + q_{i,j,k-1/2} + q_{i,j,k+1/2} + w_{i,j,k} =$$

$$SS_{i,j,k}\, \Delta h_{i,j,k}/\Delta t\, (\Delta x_i \Delta y_j \Delta z_k) \tag{8}$$

After merging and rearranging equations (2,3,4) and also grouping all the head (h) terms, the resulting equation is

$$CZ_{i,j,k-1/2}(h^{m}_{i,j,k-1}) + CX_{i-1/2,j,k}(h^{m}_{i-1,j,k}) + CY_{i,j-1/2,k}(h^{m}_{i,j-1,k}) + [-CZ_{i,j,k-1/2} - CX_{i-1/2,j,k} - CY_{i,j-1/2,k} - CZ_{i,j,k+1/2} - CX_{i+1/2,j,k} - CY_{i,j+1/2,k} + P_{i,j,k} - Sc1_{i,j,k}/(t_m - t_{m-1})]h^{m}_{i,j-1,k} + CZ_{i,j,k+1/2}(h^{m}_{i,j,k+1}) + CX_{i+1/2,j,k}(h^{m}_{i+1,j,k}) + CY_{i,j+1/2,k}(h^{m}_{i,j+1,k}) = -Q\ i,j,k - SC1\ i,j,k\ h\ m\text{-}1i,j,k/(t_m - t_{m-1}) \tag{9}$$

C represent the product of grid dimension and hydraulic conductivity = KA/L, simply conductance between nodes.

Equation (9) can be expressed for each variable head cell in the aquifer as a system of equation expressed in matrix form as,

$$[C](h) = (q) \tag{10}$$

3.4.4 Conductance. From the above and simplified equation it is easy to understand that MODFLOW processing is a matter of hydraulic head and conductance. This simplified concept is applied for all other boundary conditions in determining flow direction to or from a cell. For example; for boundary conditions such as river or stream, first their spatial locations are specified. Then, river sink or source is determined from the stage measured at that point. Hence, using equation 2 the boundary condition can be represented as;

$$q = C\,(h_s - h_c) \tag{11}$$

q = flow to the cell;

C = conductance between the cell and source/sink

h_s, h_c = potentiometric head in the sink/source and cell respectively. For higher stage in the river flow is towards the cell, otherwise the river is considered as sink.

3.5 MODPATH

Based on MODFLOW solution of groundwater flow equation MODPATH, the post processing program does particle tracking procedure. The particle tracking model PMPATH uses a semi-analytical particle tracking scheme (Pollock, 1988) to calculate groundwater paths and travel time. Once groundwater flow equation is solved by MODFLOW and hydraulic head distributions are obtained, volumetric flow rate across each cell face is calculated using Darcy's law (Q = K.A. Δh).

The average velocity components are obtained by;

$$V_{x1} = q_{x1} / (n.\Delta y.\ \Delta z)$$

$$V_{x2} = q_{x2} / (n.\Delta y.\ \Delta z)$$

$$V_{y1} = q_{y1} / (n.\Delta x.\ \Delta z)$$

$$V_{y2} = q_{y2} / (n.\Delta x.\ \Delta z)$$

$$V_{z1} = qz_1 / (n.\Delta x.\ \Delta y)$$

$$V_{z2} = qz_2 / (n.\Delta x.\ \Delta y) \quad n \text{ - porosity} \tag{12}$$

Given the starting location and time of the particle, velocity component are expressed by;

$$V_{x(t1)} = I_x(x-x_1) + v_{x1}$$

$$V_{y(t1)} = I_y(y-y_1) + v_{y1}$$

$$V_{z(t1)} = I_z(z-z_1) + v_{z1} \qquad (13)$$

I_x represents velocity gradient = $(V_{x2} - V_{x1})/\ \Delta x$

Particle acceleration at point p in x- direction is expressed by,

$$\frac{\partial v}{\partial t} = \frac{\partial v}{\partial x} \cdot \frac{\partial x}{\partial t} \qquad (14)$$

Analytical integration yields; $\ln [\,] = I_x.\Delta_t$ (15)

$V_{x(t1)}$

After time step Δt, particle velocity can then be evaluated as;

$$V_{x(t2)} = V_{x(t1)} \cdot e^{(Ix.\Delta t)} \qquad (16)$$

This can be re organized to

$$x_{(t2)} = \frac{V_{x(t1)} \cdot e^{(Ix.\Delta t)} - V_{x1}}{I_x} + x_1 \qquad (17)$$

The possible time that required by a particle to reaches exit point (in our case constant head cells, main streams and outside of the watershed boundary) is then computed. The model, then considers the direction that takes the shortest time as the exit route. MODPATH helps to executes capture zone of wells. We used MODPATH here only to process velocity distribution and travel time of particles and compare with MT3D model.

3.6 MT3D

MT3D is a comprehensive three dimensional numerical model for simulating solute transport in complex hydrogeological formations. The computer program of the MT3D transport model uses a modular structure similar to that implemented in U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model, MODFLOW (McDonald et al.

1998). Moreover; MT3D simulation start with MODFLOW simulation for that it creates a special flow file that MT3D uses to compute flow velocity and flow rate from and into neighboring cells. The partial differential equation describing three-dimensional transport of contaminants in groundwater is;

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial xi}\left(Dij \frac{\partial C}{\partial xj}\right) - \frac{\partial}{\partial xi}\left(Cvi\right) + \frac{qC}{\Theta} + \sum R \qquad (17)$$

Where:

C, Concentration
Dij, Hydrodynamic dispersion coefficient (L^2/T)
t, time
q, volumetric flux of water per unit volume of aquifer representing source or sink (1/T)
Θ, porosity
v, seepage velocity (L/T)
R, chemical reaction term

3.6.1 Solution techniques. MT3D has a comprehensive set of options and capabilities for simulating advection, dispersion/diffusion, and chemical reactions of contaminants in groundwater flow systems. The model program uses a modular structure similar to that implemented in U. S. Geological Survey modular three dimensional finite-difference groundwater flow model referred to us MODFLOW, (McDonald and Harbaugh, 1988). The numerical solution in MT3D is mixed Eulerian-Lagrangian method. The Lagrangian part of the method, used for solving the advection, employs the forward tracking methods of characteristic (MOC), the back-ward tracking modified method of characteristic (MMOC), or hybrid of these methods while, the Eulerian part of the method used for solving the dispersion and chemical reaction terms, utilizes a conventional block-centered finite-difference method (Zheng, 1990). In our case, the hybrid of both methods, Hybrid Method of Characteristic (HMOC) has been used to solve the advection part. It combines the strength of both methods providing more accurate solution for sharp and non-sharp concentration fronts. Upstream finite difference method is applicable in non advective transport dominant flow that lead to numerical dispersion; hence we did not used in this report.

3.6.2 Advection term. Solute transport in groundwater is mostly dominated by the advection term. The term also describes velocity of transport is equal to groundwater velocity. HMOC in the automatic adoption procedure implemented in MT3D; when sharp concentration fronts are present, the advection term is solved by the forward tracking MOC, away from such fronts, the term is solved by MMOC (Zheng, 1990). This automatic switching between the two methods is controlled by the relative concentration predefined gradient (0.01). The MOC solves the advection term with the set of moving particles by eliminating numerical dispersion in sharp front situation and MMOC approximates by tracking the nodal points of fixed grid backward in time using interpolation technique. However, when the front drive away by dispersion the forward tracking stops and the corresponding particles are removed.

3.6.3 Dispersion term. The concentration change due to dispersive is solved fully explicit central finite-difference method. To retain a stability criteria associated with this scheme, transport step size cannot exceed an upper limit (Bear, 1979) defined by equation,

$$\Delta t \leq \frac{0.5\ R}{\dfrac{D_{xx}}{\Delta x^2} + \dfrac{D_{yy}}{\Delta y^2} + \dfrac{D_{zz}}{\Delta z^2}} \qquad (18)$$

where Δx, Δy and Δz are the widths of the cell in the x, y and z-directions; R is the retardation factor. The components of the hydrodynamic dispersion coefficient Dxx, Dyy and Dzz are calculated by;

$$D_{xx} = \phi_l \frac{V_x^2}{|V|} + \phi_{ht} \frac{V_y^2}{|V|} + \phi_{vt} \frac{V_z^2}{|V|} + D^*$$

$$D_{yy} = \phi_l \frac{V_y^2}{|V|} + \phi_{ht} \frac{V_x^2}{|V|} + \phi_{vt} \frac{V_z^2}{|V|} + D^*$$

$$D_{zz} = \phi_l \frac{V_z^2}{|V|} + \phi_{vt} \frac{V_x^2}{|V|} + \phi_{vt} \frac{V_y^2}{|V|} + D^* \quad (19)$$

Where:

ϕ_l [L] is the longitudinal dispersivity;

ϕ_{ht} [L] is the horizontal transverse dispersivity;

ϕ_{vt} [L] is the vertical transverse dispersivity;

vx, vy, vz [L/T] are components of the flow velocity vector along the x, y, and z axes; $|v| = (V_x^2 + V_y^2 + V_z^2)^{1/2}$

3.6.4 Sink and source term. This term represents solute mass dissolved in water that either, entered the simulation domain from source, or leaving the domain. Pollutant source can be either, distributed over the watershed area that includes recharge and evapotranspiration or, point source includes wells, drains and rivers. Constant head and general head dependent boundaries in the flow model are also treated as point sources or sinks because they function in exactly same way as wells, drains, or rivers in the transport model (Zheng, 1990). Point sources of constant head and spillage were considered to indicate fate of contaminants for both scenarios. This helps to assume industrial releases and breakdown of sewerage system. Chemical reaction term was not considered in this particular case as we model fate of metals.

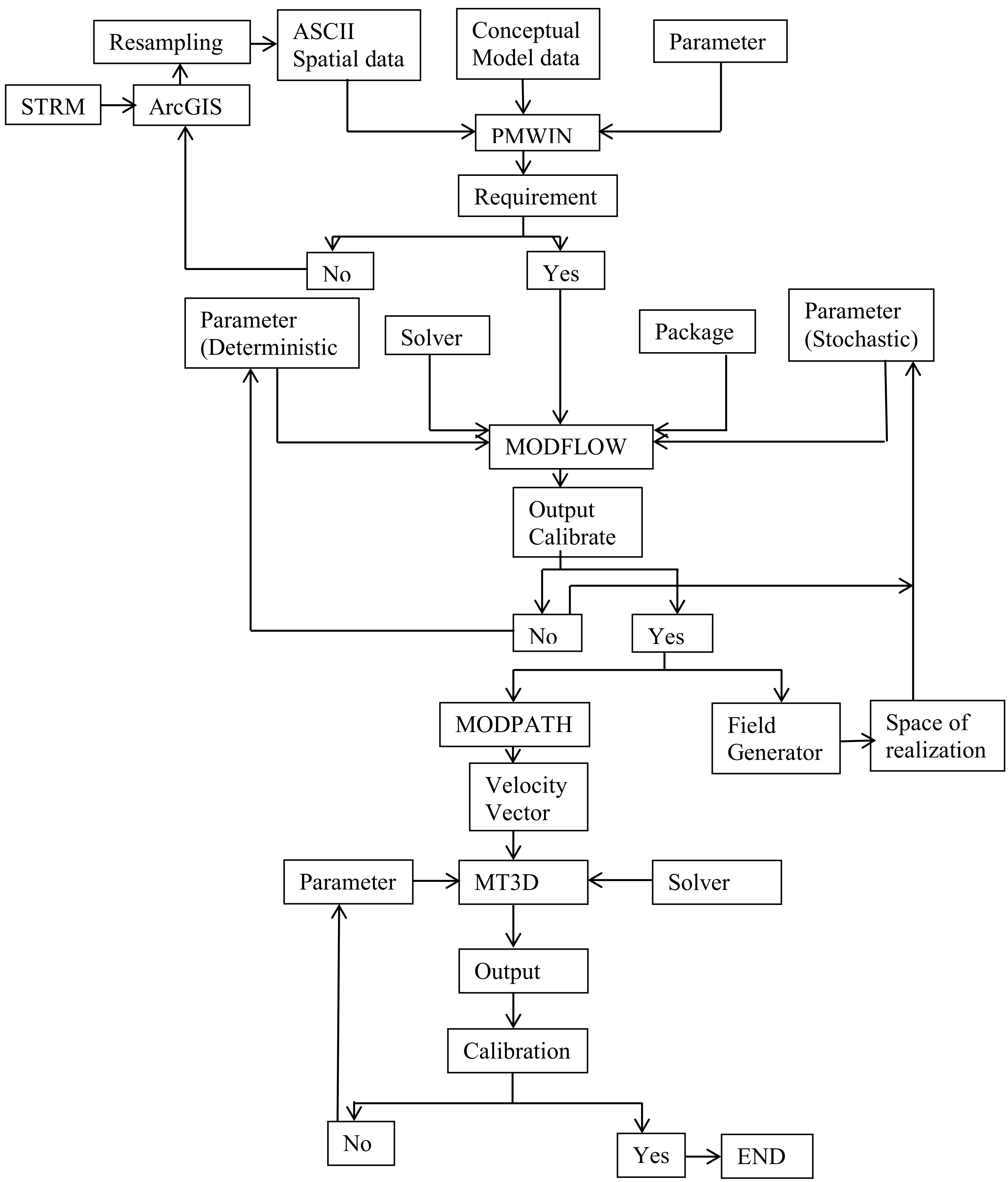


Figure 4 Flow chart of modeling

CHAPTER 4

Results and Discussions

4.1 Integration of Conceptual and Numerical Model

4.1.1 Grid setting and discretization. As discussed in section 2.3.2, regolith layers consist of loose, heterogeneous material that includes dust, soil, broken rock and also other materials. It underlain by fractured bedrock. The transition layer similarly consists of particles range in size from silt and clays to large boulders of unweathered bedrocks. For this particular model, the variable depth of the transition zone is averaged to about 3 m and amalgamated to the overlaying layer, regolith. Consequently, we categorized our model as single layered unconfined aquifer.

The governing equation is underpinned by the assumption that the principal direction of the hydraulic conductivity tensor is coincident with the coordinate axis of the model (Anderson et al., 1992). Except Buffalo Creek Watershed, that aligned approximately southwest-Northeast, all other adjacent watersheds (Troublesome, Haw River and Little Almanca) approximately aligned east-west, Figure 7.

The general grid orientation then rotated 19^0 clockwise in the direction of hydraulic conductivity tensor, Figure 6b. Grid boundary is set to fit the natural watershed boundary as developed by ArcGIS. The surrounding cells outside the grid were set as no flow cells. Orientation of the grid was made to follow the general trend of groundwater flow direction.

The discretization package also sets the spatial and temporal dimensions. From ArcGIS processed and resampled data, we finally assigned a constant horizontal grid dimension of 200 m x 200 m (width x length) organized along rows and columns. With this dimension, the watershed has been discretized into a total of 10,496 cells arranged into 128 columns and 82 rows, Figure 6a.

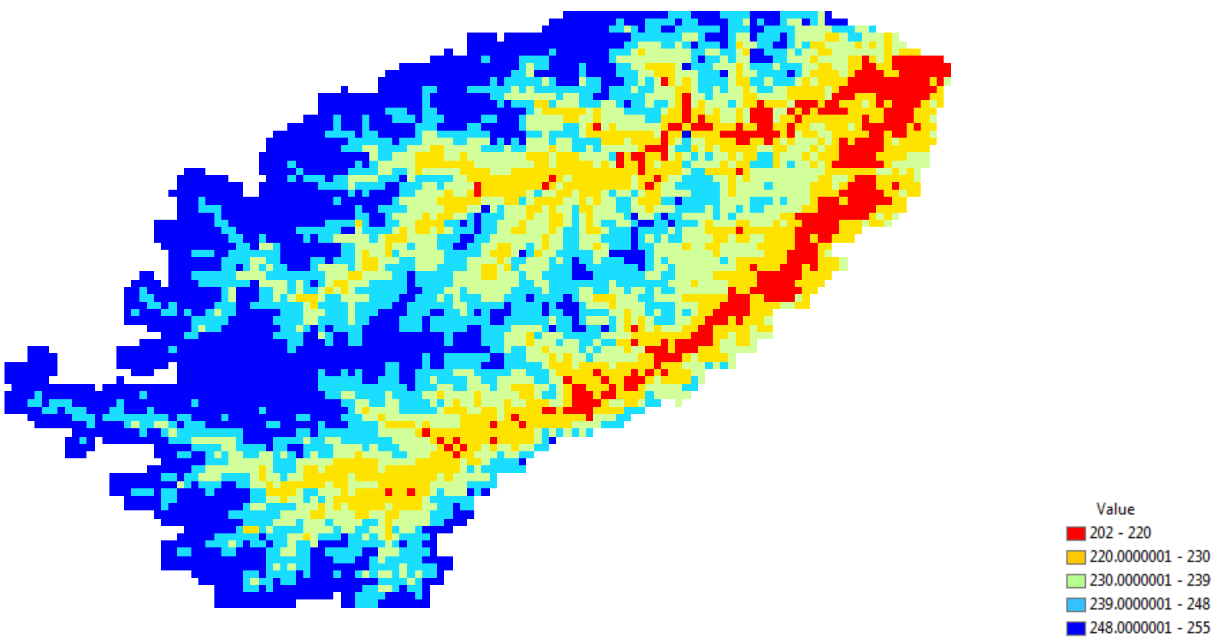
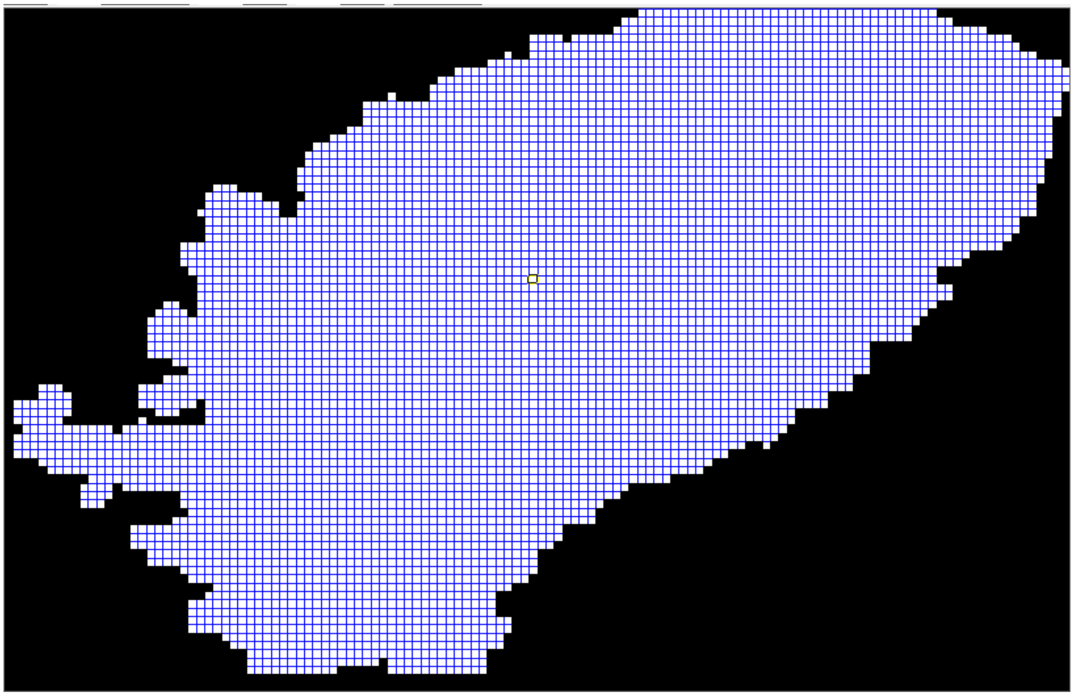
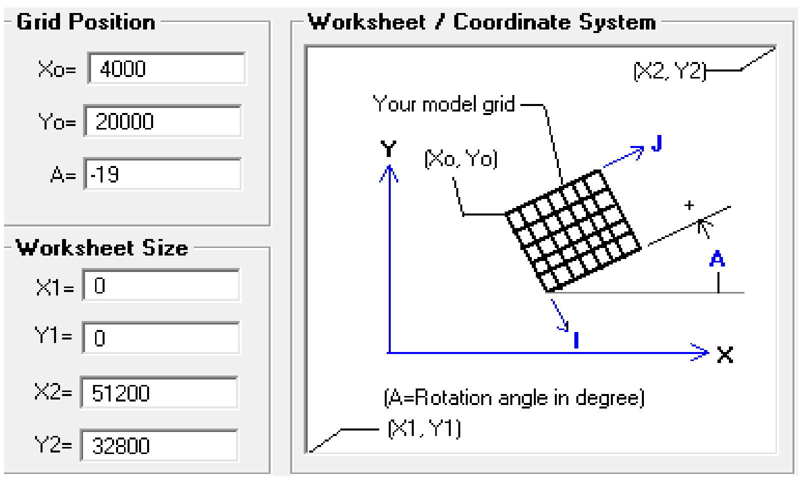


Figure 5 ArcGIS resampled and delineated DTED for Buffalo Watershed



(a)



(b)

Figure 6 a) Discretized watershed mesh (200m x 200m) and, b) orientation of the grid mesh

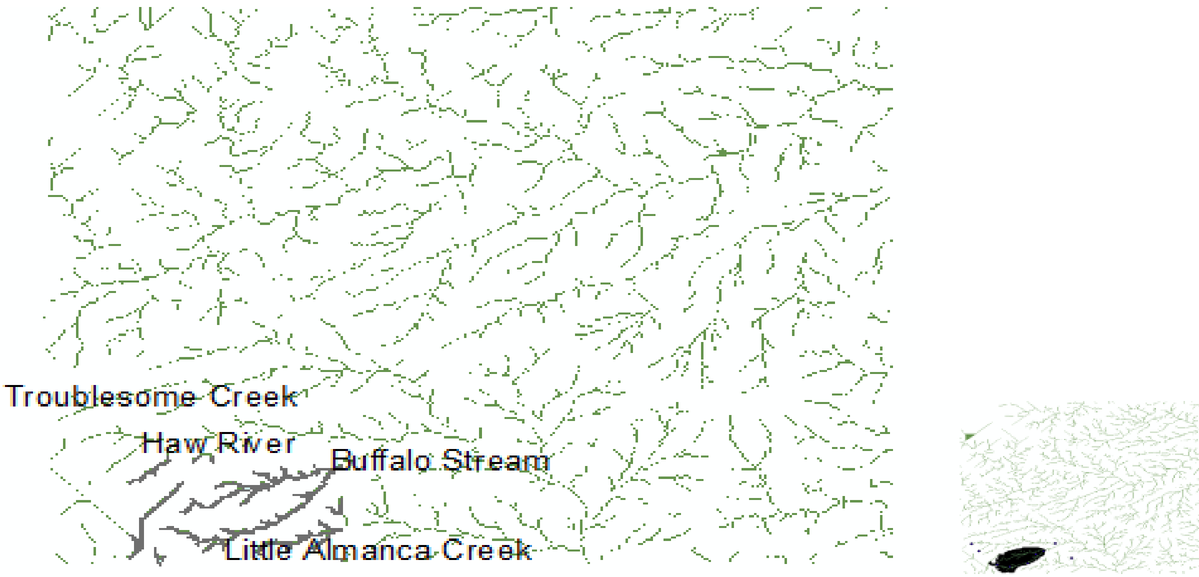


Figure 7 Local drain network map of parts of upper cape fear drainage; river boundary line developed from river segment shape files of ArcGIS

MODPATH and MT3D models require the actual top and bottom elevations of the discretized watershed to process particle tracking and solute transport, respectively. GIS processed, resampled and extracted surface elevations, Figure 11 of the entire watershed were imported to the grid (top of layers) of the PMWIN menu after converting it to the appropriate ASCII format. Each of the elevation value represents the corresponding 200 m x 200 m area of the discretized watershed surface elevation. The extent of surface and groundwater sheds usually does not coincide. It is difficult to identify groundwater shed extent, simply because it is not visible from a surface. In general, the physical extent of watershed can be very different from that of the underlying aquifer (Winter et al., 2003). However, for shallow unconfined aquifers like Buffalo Creek, there is a great coincidence that the surface watershed boundaries define also aquifer extent. Conventional approaches to groundwater modeling use the outer watershed boundary as the maximum extent of the model domain. The model boundary definition assumes that groundwater catchment boundaries directly coincide with the surface water catchment area

(Sykes et al., 2006). Hence, the horizontal extent of the aquifer is defined similar to the shape of surface watershed boundary.

The vertical extent of the regolith aquifer varies from place to places. As mentioned by Daniel, (1989) and from well log reports by Nutter and Otton (1969), the average estimated depth of the regolith is 52 feet (15.85 m). Thus, the final averaged thickness of the aquifer including the transition zone (see sections 2.3.2 and 4.1.1) is estimated to 18.14 m. Considering this depth as surrogate aquifer thickness, an imaginary plane was constructed parallel to the ground surface slope so that, individually discretized cell's thickness can be determined. In the meantime, depths of a few grid cells were reduced to zero in the stream channel bed. This indicates that the total channel down cut fully penetrates the aquifer. The upstream reaches have eroded down to the bed rock at several riffles; within the project reach station 5556 is also located at bedrock outcrop (Matthews, 2002). Thus, each of the discretized aquifer cells (blocks) is set to a depth varying from 5.65 m to 48.05 m. Daniel (1989), thickness of the regolith throughout the study area is extremely variable and ranges from zero to more than 150 feet. For all spatial and temporal data required by MODFLOW/PMWIN packages, an ASCII character coding type input were defined with strict format. Ground surface elevation values, then imported to the model grid after processed and transformed to ASCII format from GIS as mentioned in (section 3.2).The total grid is divided into 5743 active, and 4753 inactive cells.

4.1.2 Parameters. MODFLOW requires an initial hydraulic head input. Due to significant variability of surface elevations, reference surface is taken from grid bottom elevation to assumed initial hydraulic head values. We employed manual trial and error procedure, and assumed initial hydraulic head values for each block cells to 5 m above their assumed corresponding bottom elevation. Based on field and laboratory tests (see sections 2.3.3 and 2.3.4), an initial effective porosity value of 0.3 and horizontal hydraulic conductivity value of 6.9

x 10^{-6} m/second was assigned for all grid cells. For all parameters and steps, time unit of second is used for modeling.

4.1.3 Stream networks and hydraulics. The stream flow-routing package in PMWIN can be categorized into four major types of conceptualized elements representing stream components namely; reach and segment, stream channel, flow and channel hydraulic conductivity. The main channels and tributaries of North and South Buffalo streams were defined in stream flow routing package as shown in, Figure 8a. The stream-flow routing package is designed to account for the amount of flow in streams and simulate the interaction between surface stream and groundwater (Prudic, 1989). Initially; the extent and distribution of the stream network were determined using ArcGIS tools from its original 30 m x 30 m horizontal grid to the resampled size of 200 m x 200 m (see section 3.2).

Reach corresponds to individual cell in the finite-difference grid and is assigned with a specific number, reach number. Reach number is a sequential number in a segment that begins with one for the farthest upstream reach and continues in downstream order to the last reach in the segment, Figure 9. A segment consists of a group of reaches connected in downstream order. Stream flow is accounted for by specifying flow for the first reach in each segment and then computing stream flow to adjacent downstream reaches in each segment as inflow in the upstream reach plus or minus leakage from or to the aquifer in the upstream reach. The accounting scheme used in this package assumes that the stream flow entering the model reach is instantly available to downstream reaches (Chiang et al., 1996). In PMWIN, MODFLOW recognizes a maximum of 25 numbers of segments. In addition, each segment can only have a maximum of 10 tributaries along its all length. Consequently, a total of four smaller tributaries streams (three along north buffalo and one south buffalo) were omitted from stream structure, Figure 8a and 8b.

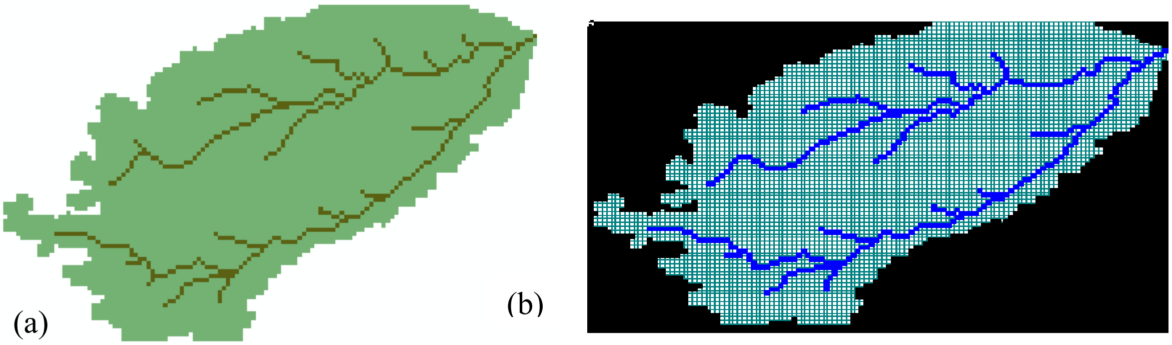


Figure 8 Stream network and distribution developed from (a) ArcGIS, (b) MODFLOW

Stream channel properties represent parameters (top and bottom bed elevations, width slope and manning's coefficient) required in stream flow calculations. To determine stream bed elevation along the longitudinal section of the main and tributary channel, depth of the channel cut from surface was estimated. For head segments and tributaries; a 1 m depth of cut was assumed from the point where stream channel is defined by ArcGIS and steadily increased up to 2.25 m where the next segment commences. The previous segment tail depth is then considered as the initial depth for the next downstream segment. This was continued up to the last segment and its corresponding downstream reach.

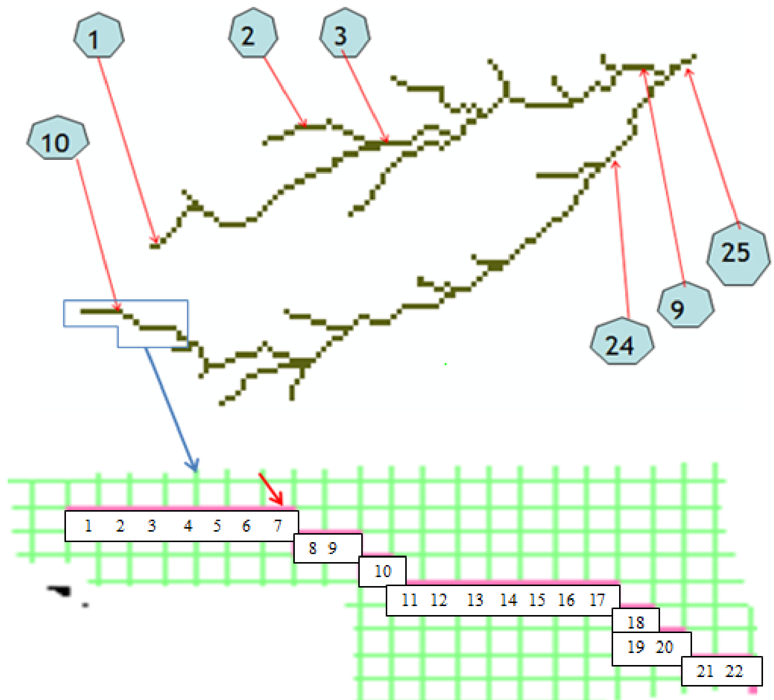


Figure 9 MODFLOW processed South and North Buffalo stream segment number and reach number (segment number 10 has 22 reaches)

Accordingly, depth of 3 m has been calculated for the last reach, reach number 7 of segment number 25. All intermediate depths were fixed by interpolating except at locations where slope changes sharply. For natural falls and steep slopes, we followed the natural trend. The stream flow package also requires the input of stream bed bottom elevation. Thickness of the streambed is also required by stream flow package. Depth from 0 up to 30 centimeters was used depending up the depth of the channel cut (section 4.1.4).

Stream's stage and discharge data (2007 – 2014) were obtained from gauging stations monitored by U.S Geological Survey. Gauging stations (USGS 02094659, USGS 02094770), (USGS 02095000) and (USGS 02095500) measure stream flow and stage of South Buffalo, North Buffalo and Buffalo streams respectively. The average annual depth of flow for South Buffalo stream stage near Pomona Dr. (USGS 02094659), US 220 (USGS 02094770) and near Greensboro (USGS 02095000) are 0.276 m, 0.644 m, and 0.998 m in order. The annual average stream depth of North Buffalo is 0.694 m near Greensboro (USGS 02095500). Gauging station SR2819 near McLeansville (USGS 0209553650) is located 300 feet downstream of the confluence point of both streams. The average stream stage is about 0.807 m. Essentially, this measurement data were used to validate previous calculated depths (section 4.1.4). For all other small tributaries with no measured data, average depth of the stream was set as 0.3 m.

The extent and direction of flow between surface water in the stream channel and groundwater depend on medium property and hydraulic head. As indicated in Matthew, (2002) impermeable bedrock, thin bed material and permeable bed material up to 30 cm were observed in the channels. Initial streambed hydraulic conductivity equivalent to aquifer horizontal hydraulic conductivity was assumed.

4.1.4 Wetting capability. The wetting capability allows the simulation of rising water table into unsaturated (dry) model cells. It is important when surface recharge is applied to cells and raises the water table and convert dry cells to wet. In addition, during iteration periods heads may decrease temporarily and goes dry. The wetting capability allows users to able to convert dry cells to wet back. The hydraulic head is set to the following equation;

$$H = \text{bottom} + \text{WETFACT}*|\text{THRESH}| \qquad (20)$$

H – hydraulic head at the cell

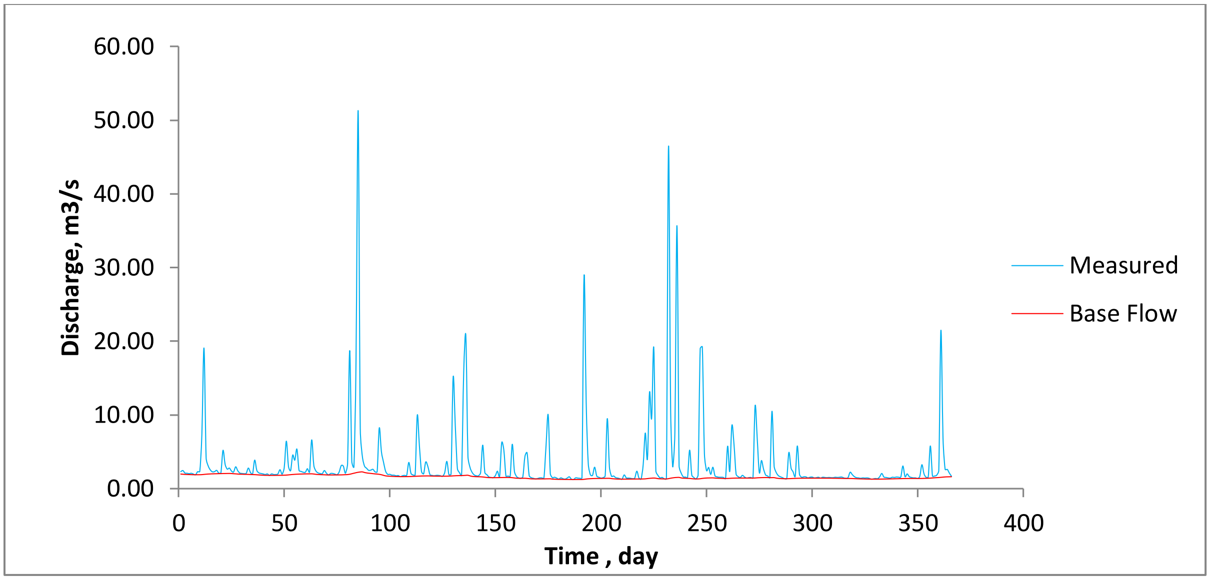
WETFACT*|THRESH| – user specified constant called wetting factor threshold

The threshold is set to a value that allows cell below the dry cell, and other four horizontal cells can cause the cell to become wet. Moreover; for the unconfined aquifer horizontal conductance between cells is a function of head so that all the neighboring cells updated during the solution process.

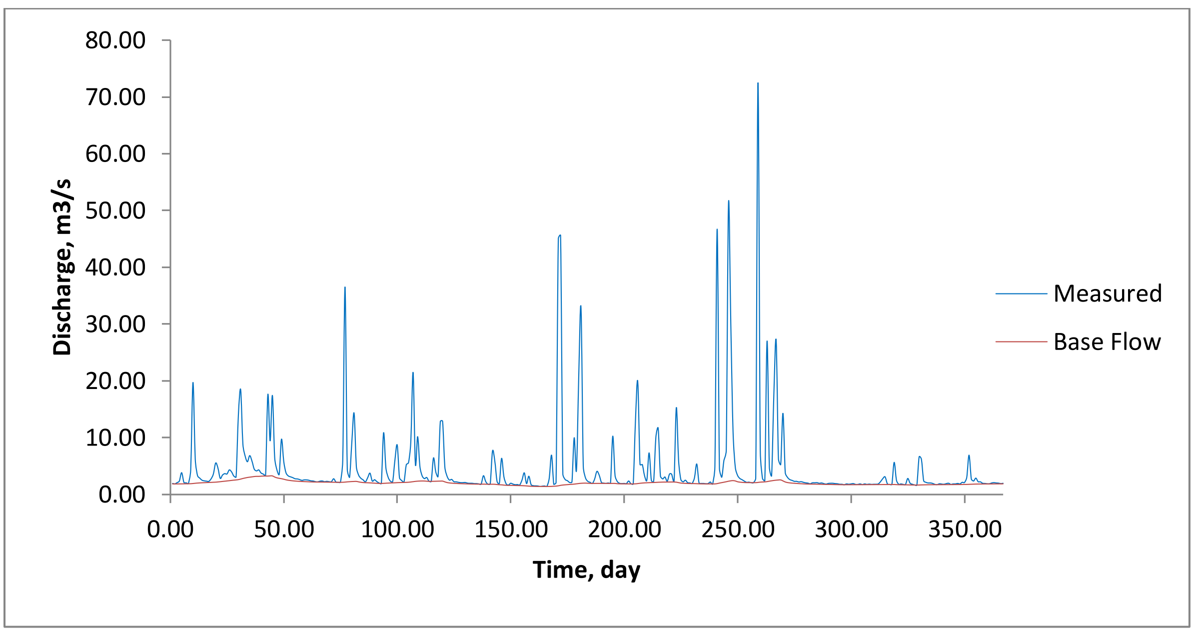
4.1.5 Solver (PCG2). The preconditioned Conjugate Gradient (PCG2) has been used to solve an iterative method to solve a matrix equation of groundwater described in section (3.4.1.3). It works well, because the required iteration parameters are calculated internally and need not be estimated (Hill, 1990).

4.1.6 Areal Recharge and Evapotranspiration

Areal recharge rate is estimated by dividing the annual volume of water separated by filter program (Figure 10) and distributed over the watershed area of 229.214 square kilometers. Hence calculated flux rate of 2×10^{-09} m/second is used for initial input. A fixed amount of an initial value of annual evapotranspiration rate of 2.2×10^{-8} m/second is also utilized based upon previous studies and laboratory test results (section 2.3).



(a)



(b)

Figure 10 Surface runoff and base flow hydrograph for measured year, (a) 2012 and (b) 2000

4.2 Results

4.2.1 Summary. A two dimensional steady-state MODFLOW model was constructed to simulate groundwater flow for the shallow regolith aquifer, Buffalo watershed. The aquifer (unconfined aquifer type) is underlain by fractured bedrocks at different depths. The model requires the use of stream flow routing and recharge packages. In the basic package boundary conditions (weather flow in the cell is constant, variable or no flow), and initial hydraulic heads values defined. Values of hydraulic conductivity and the wetting capability are defined in the block-centered flow package. Because of the shape of the watershed, the maximum possible reduction in inactive cell could not be done more. The watershed is rotated 19^0 clockwise to follow the general trend of groundwater flow (conductivity tensor) in the upper piedmont catchment. This helps, in fact, in avoiding the drying of most of the cells while running the model. It also helps in reducing the total number of inactive cells from computation.

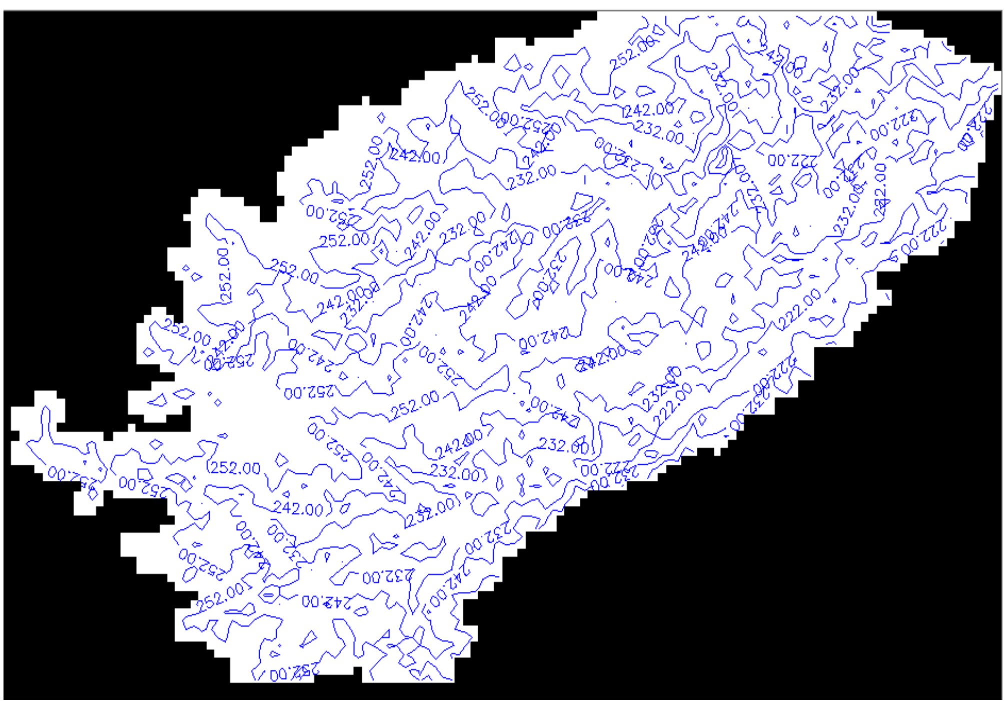


Figure 11 Contour map of Buffalo watershed surface elevation, ArcGIS processed

Model calibration involves determining parameter's magnitude and their spatial distributions. Modeling has been done in the area where limited groundwater data was available. Consequently, inverse modeling using PMWIN-PEST could not be processed. Hydraulic head distribution has been calibrated using available water table elevations of South Buffalo flood plain wells data, and the nearby wells from adjacent watersheds. Gibsonville monitoring well is the only available active well in Guilford County (Almanca watershed). It is considered for calibration through interpolation, along 10 km distance of gentle surface slope. The other monitoring well is Yow 2 (inactive well) found at about 5 km from Buffalo watershed boundary in Deep River watershed.

4.2.2 Sewage discharge. Effluent discharge; externally sourced, barely passed through natural system of the watershed, has a significant impact on parameter values unless considered properly in one of PMWIN-MODFLOW packages. Different approaches: (i) distributing the total annual flow as a recharge flux, (ii) considering the equivalent discharge as recharging well by activating well package, and (iii) assuming a river channel having an equivalent discharge. That means the river is assumed to pass through mainstream channel of North or South Buffalo coming from another headwater sheds. All these approaches were not successful. In both of the first cases, even though the model was able to run properly, values of hydraulic conductivity were un-realistic. Similarly, activation of river package was also failed to converge water budget balance. Approach (1v) that assumes the discharge as a specified constant head pool in the mainstream channels, over the modeling period was able to calibrate groundwater flow effectively. Consecutively; all grid cells of North and South Buffalo streams, identified by ArcGIS as stream channel was categorized to constant head cells, instead of being a variable head or/and stream cell, Figure 12.

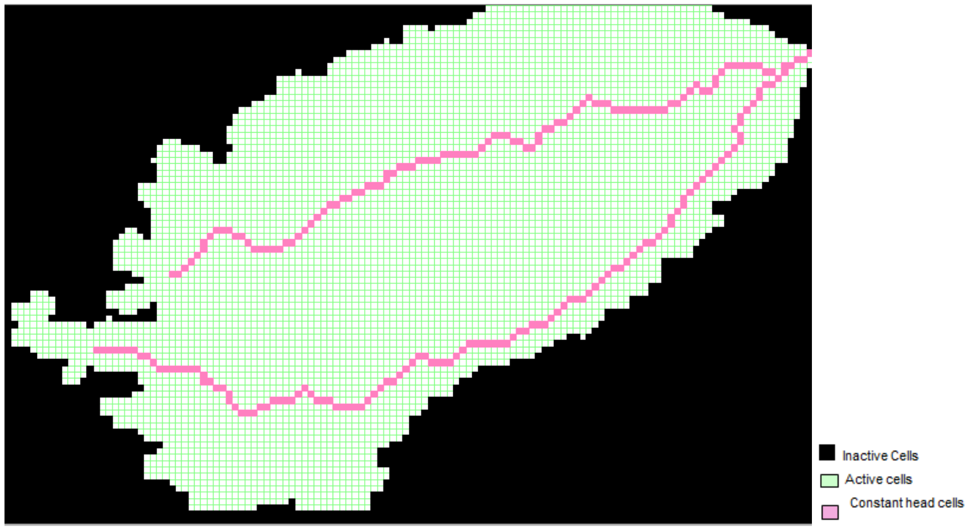


Figure 12 Boundary conditions, MODFLOW processed

This situation, particularly for North Buffalo stream agrees with its natural/existing condition. Along North Buffalo stream channel, there are a number of small lakes and polls that naturally help to regulate the flow at downstream throughout seasons of the year.

4.2.3 MODFLOW

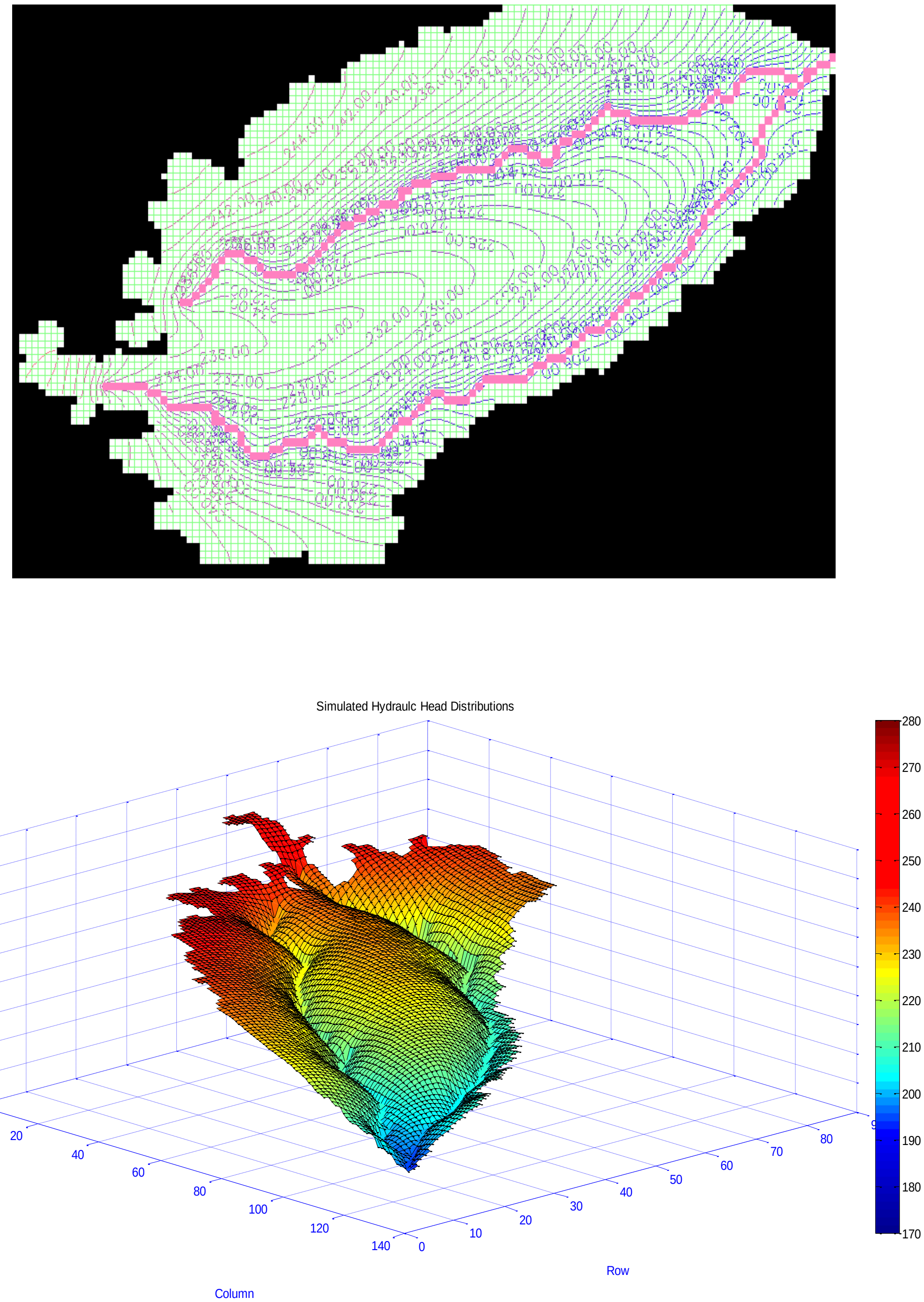
4.2.3.1 Deterministic approach. Groundwater flow system needs to be simulated and calibrated before processing solute transport model. Model calibration consists of changing input model values so that it matches with measured values within an acceptable range. We could not succeed in the initial trial and error modeling using three parameters; horizontal hydraulic conductivity, evapotranspiration and recharges flux. Parameter values continue to be very sensitive, particularly for horizontal hydraulic conductivity and evapotranspiration rates. For any slight changes in horizontal hydraulic conductivity (value such as 10^{-10}), the net volumetric water budget (inflow - outflow) changes to nearly 62 %. In most of the grid cells, hydraulic head outputs went to elevations beyond the land surface, and most of the cells went dry while we change evapotranspiration rate to the order of 10^{-08}.

We tried inverse modeling approach using PEST (parameter estimator). This inverse modeling tool configured in PWMIN and run outside of MODFLOW model. It helps to estimate horizontal hydraulic conductivity, evapotranspiration and recharge rate. Unfortunately; PMWIN recognizes only active wells from within the watershed. The nearest available wells from neighboring watersheds are; Gibsonville (G 50W2) and Yow 2 monitoring wells. Gibsonville is an active monitoring well. It is located at about 10 km from Buffalo watershed boundary at the real-world coordinates of latitude 36.088262 and longitude 79.547915. On the other hand, Yow 2 is inactive well located at 5 km from southern water divide line, latitude 35.958388 and longitude 79.838645. We tried to idealize and locate both monitoring wells inside Buffalo watershed, systematically. Image wells were transformed, using watershed boundary as a center of rotation to similar altitude in Buffalo watershed. Eventually, both wells were used to calibrate the hydraulic head with logic and some assumptions for the fact that PMWIN does not read wells unless they are active and real.

Back to the trial and error procedure, we decided to reduce the number of parameters for estimation because results could not be converged. Accordingly, the previous recharge flux that includes the component of evapotranspiration is removed from the input data. While doing so, the annual net groundwater recharge documented in U.S. Geological Survey (Daniel et al., 1998) has been used as an initial input and verified with the net base flow we separated (Figure 10). For this particular case, seasonal variations of groundwater depth in Guilford County and adjacent Counties were also reviewed to estimate the annual recharge flux. This net recharge flux was estimated from the annual average base flow that groundwater contributes to the stream. While doing so, it is estimated that base flow from the catchment has no any other source than areal recharge (section 2.6).

Steady state calibration was set for stress period of 15 years divided into 100 time steps. Major outputs of MODFLOW; hydraulic head distribution, Figure 13 and water budget balance were compared with measured data. MODFLOW model water budget balance output was about

0.0007 percent (Inflow – outflow), indicating the numerical efficiency of the model. A discrepancy of 3.4 percent is observed in volumetric difference of MODFLOW output and annual measured base flow. This same annual volume was distributed over the entire watershed and found that, the net recharge rate raises groundwater table by 0.0496 m, until it emerges as base flow compared to previous assumptions, 0.0511 m (section 3.3). Discrepancy of 2.9 percent is considered good agreement. Calibration of hydraulic head with available groundwater depth data showed consistent agreement Figure 19.



(a)

(b)

Figure 13 Calibrated hydraulic head distribution in deterministic approach), (a) contour map, (b) three dimensional views

4.2.3.2 Stochastic approach. The framework of stochastic analysis was developed to address the role of natural variability and its influence on subsurface processes (Ruskauff, 1998). Field and laboratory test results of hydraulic conductivity indicates variation in the order of kilometers. These variations, in fact, can be encountered within meters and centimeters distance both vertically and horizontally. Hydraulic conductivity varies by up to five orders of magnitude over a distance of less than a meter vertically and about 100 meters horizontally (Gego et al., 2011). Laboratory and field results indicate that aquifers are generally nonhomogeneous. In heterogeneous aquifer, seepage velocity is no more constant and also follows curvilinear motion. This variability, in space and time, are, in fact, random. Consequently, if the general groundwater flows equation represents randomly distributed parameters then, solution of groundwater flow and contaminants transport are defined through statistical approach. It also helps to simulate effects of small scale variations of known and unknown parameters of the aquifer.

Using Field Generator tool in PMWIN, we generated horizontal hydraulic conductivity values of heterogeneously distributed. Parameter value for each model cell is interpolated from the measurements using the Kriging's method.

The correlation length is determined from the measurements.

$$y(x) = \mu + Z(x) \tag{21}$$

x – an m dimensional vector

μ - is a constant global model

Z(x) – represent a local deviation from the global model

Following data were utilized to generate statistically distributed hydraulic conductivity realizations.

Measured (average) value = 3.472673×10^{-05} m/sec.

Number of realization = 25

Mean value in log scale, μ = -4.588

Standard deviation = 0.5 (1.04×10^{-4} m/sec.)

Hydraulic conductivity and transmissivity are commonly assumed to be lognormally distributed (PMWIN). Representing hydraulic conductivity by K, variable X with a mean value μ and standard deviation σ has lognormal distribution, X = log (K) from its original distribution see Figure 14.

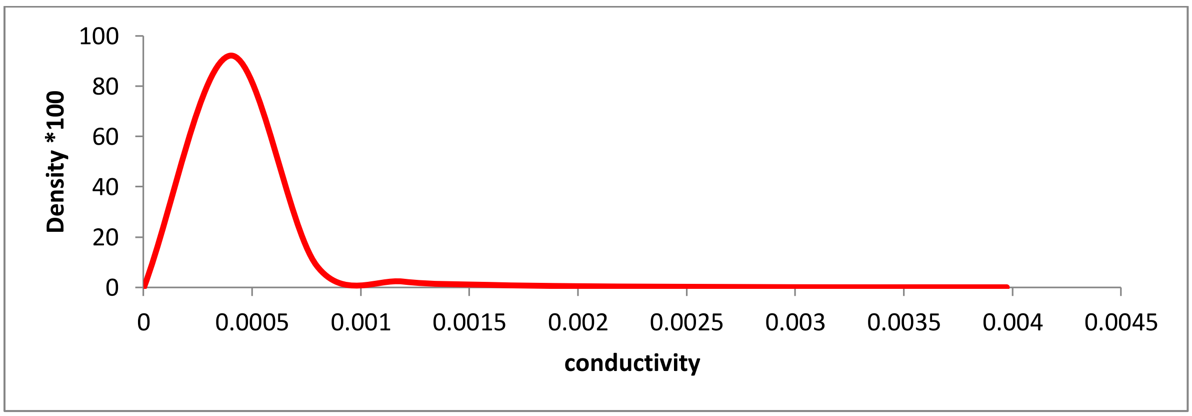


Figure 14 Sample original scale of generated horizontal hydraulic conductivity distribution

Conditional simulation, in which existing measurement data are used to reduce space of realization, was performed. The mean value of 10^{-4}, Table 1 and standard deviation of 0.5, a constant correlation length of 0.2 were calibrated and used to generate matrixes of horizontal hydraulic conductivities. A total of 83, 968 different hydraulic conductivity matrix values in 8 sets were able to calibrate the model Figure 15. Realization outputs are saved in ASCII matrix format. Out of these realizations, eight were selected as best results in respect to their hydraulic head distribution results as compared with measured values and also with outputs having minimum number of cells went dry for the selected fifteen years of the stress period, Figure 16.

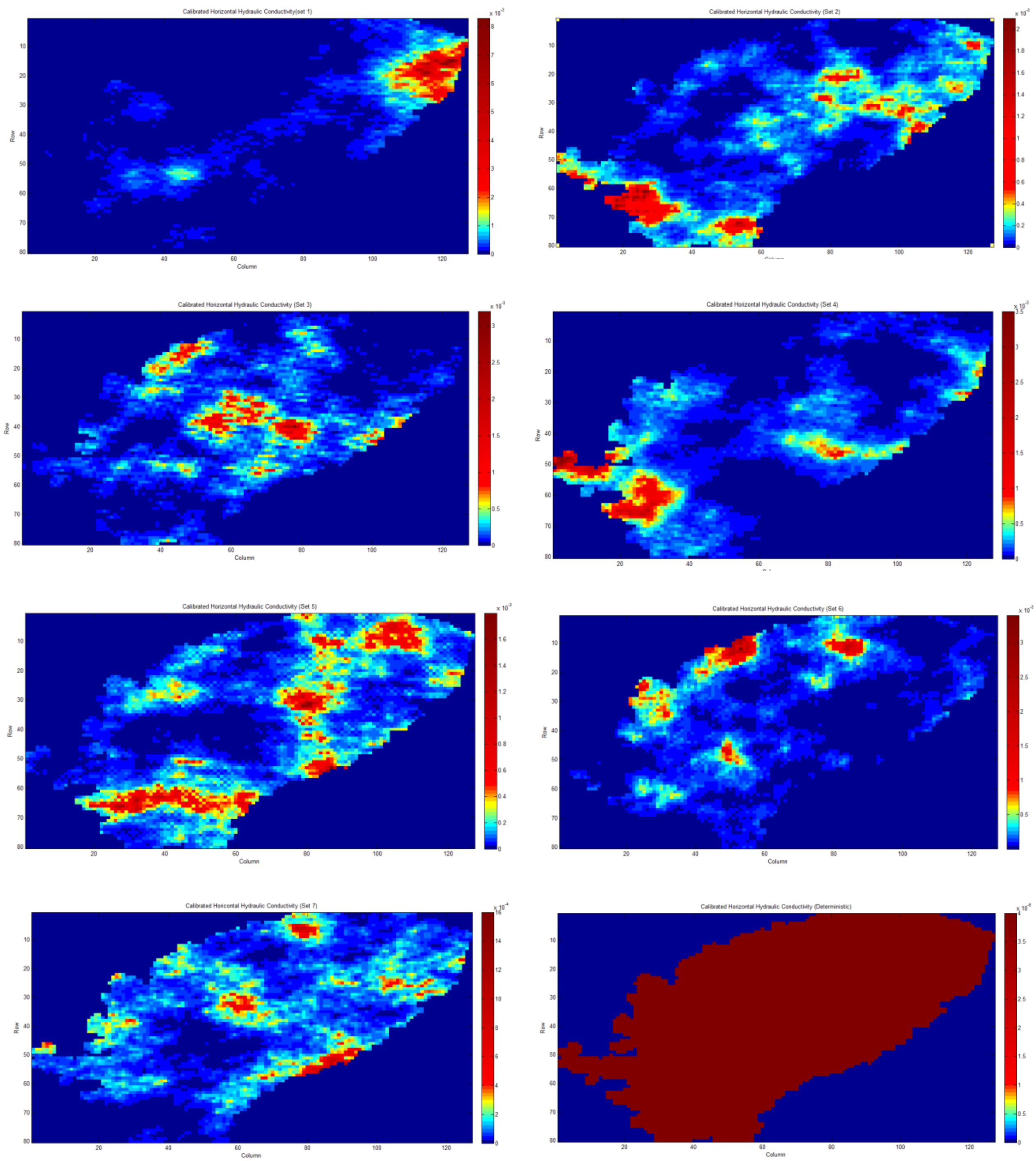


Figure 15 Stochastically distributed and calibrated horizontal hydraulic conductivity sets

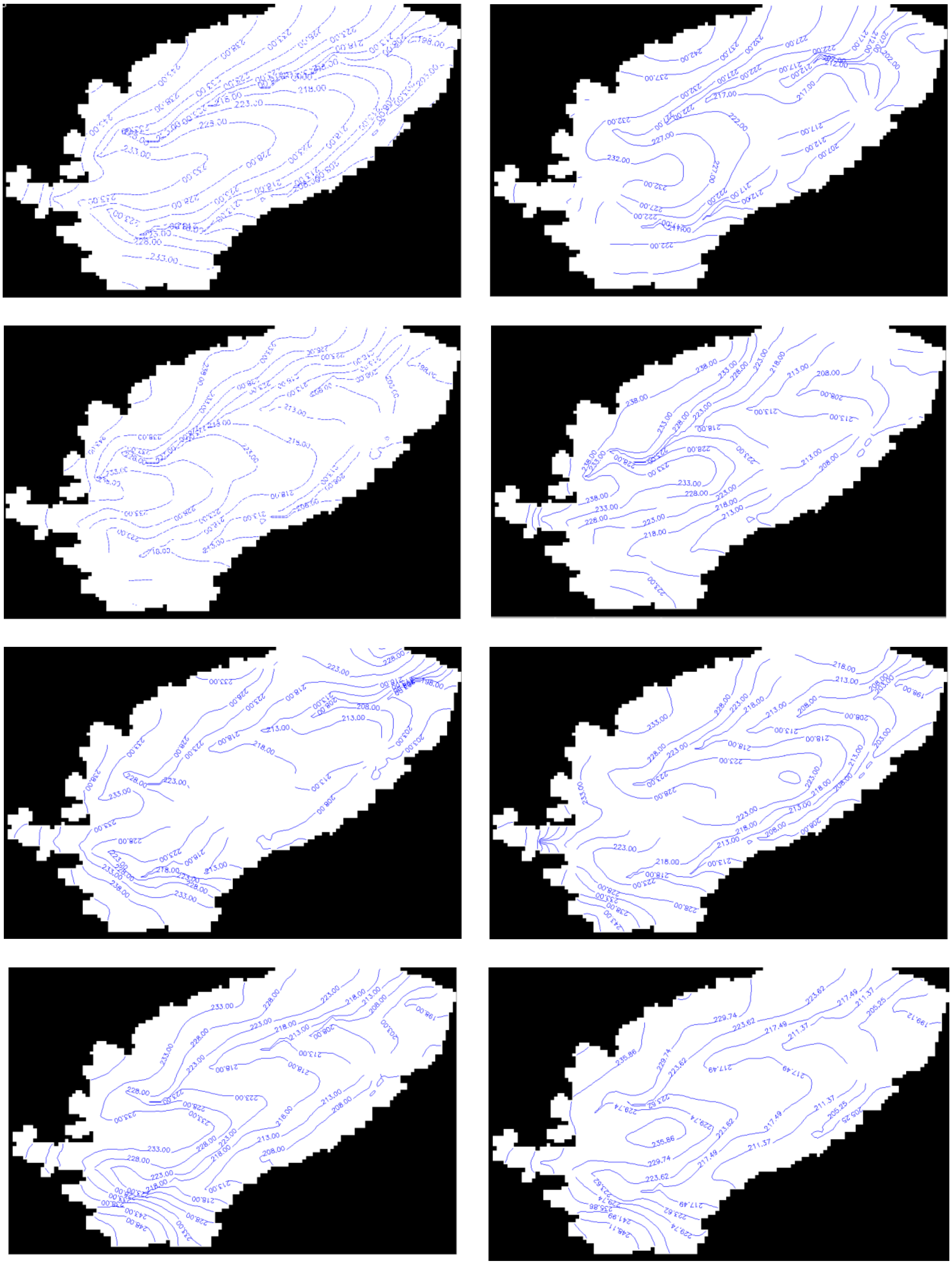


Figure 16 Stochastically calibrated hydraulic head distribution sets throughout the watershed

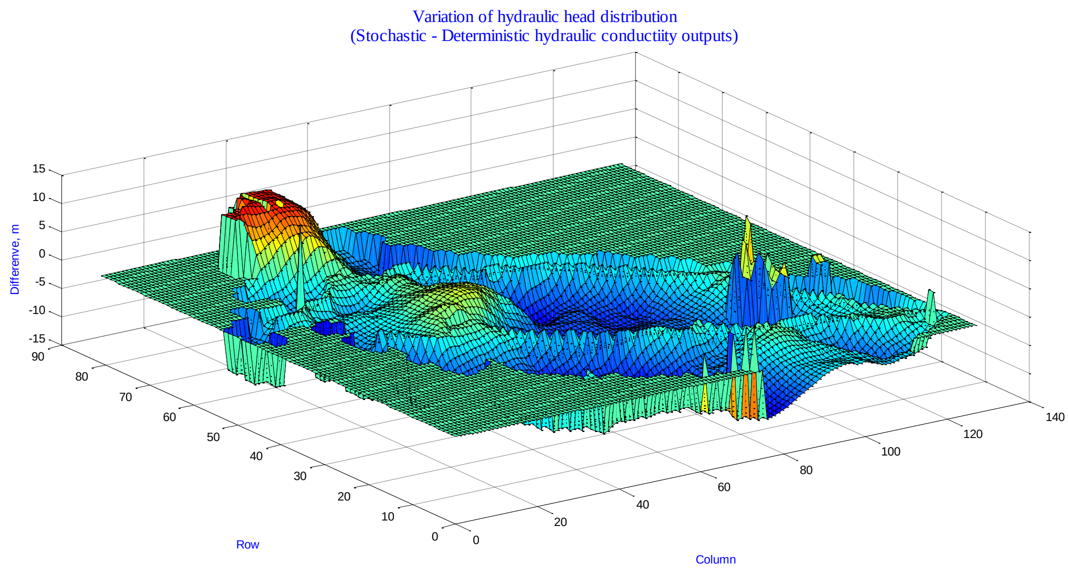


Figure 17 Groundwater depth difference (Deterministic – Stochastic) across all grid cells

Table 1

Summary of horizontal hydraulic conductivity and flow velocity

	Calibrated hydraulic conductivity, m/sec			**Calibrated flow velocity, m/sec**		
Set	**maximum**	**Minimum**	**Average**	**Maximum**	**minimum**	**Average**
set 1	1.56E-03	4.00E-06	1.09E-04	1.49E-05	2.51E-11	7.27E-07
set 2	2.10E-03	3.37E-06	1.88E-04	3.39E-05	3.05E-10	7.89E-07
set 3	3.18E-03	8.03E-07	1.44E-04	2.69E-05	5.29E-10	8.50E-07
set 4	3.47E-03	4.31E-06	3.00E-04	2.69E-05	3.12E-10	8.54E-07
set 5	1.77E-03	2.64E-06	1.50E-04	6.55E-05	8.49E-15	1.15E-06
set 6	3.39E-03	2.25E-06	1.29E-04	1.41E-05	2.33E-10	8.13E-07
set 7	1.56E-03	4.00E-06	1.09E-04	5.78E-05	3.66E-11	2.77E-07
set 8	8.30E-03	1.93E-06	4.02E-04	3.08E-05	6.07E-10	6.09E-07

***4.2.3.3* Calibration.** Local and regional scaling was employed in the calibration process. The local scaling focused on the available measurements within the watershed. Regional scaling relates the aquifer in a horizontal dimension; that includes assessment of piedmont and/or

Guilford County groundwater measured data, Figure 18. It helps to compare our results vis-à-vis to the regional trend of groundwater movement.

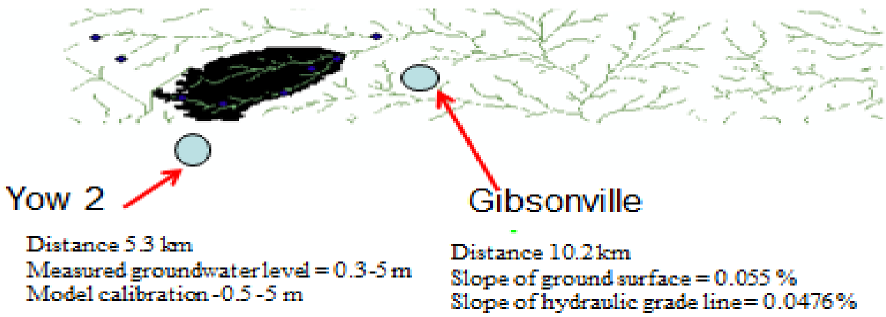


Figure 18 Regional scale calibration target wells distance and location

Model results of spatial hydraulic heads distributions are compared and verified with the available information and previous studies as discussed (section 2.4). The geographical location of water table wells of South Buffalo wetland (36^0 2' N and 79^0 49' W) overlaps with cell grid on either side of stream segment number 12, reach number 10. For this particular area, steady state calibrated groundwater depth was 5 m and 7 m from the ground surface on either sides of the channel. However, the simulated result of hydraulic heads in flood plain region varies from some few centimeters above (inundation) to, 7 m below the ground surface. Here, comparison with the latter case makes sense; for that the surrounding hydraulic head average represents the weighted average distribution for the surrounding grid cells of the flood plain. Correlation coefficient, R-squared value of 0.7471 was considered good fit, Figure 20

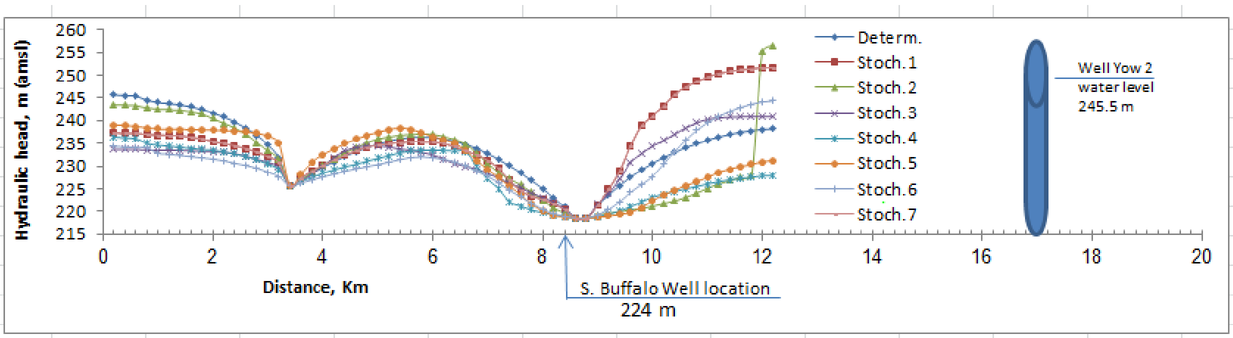


Figure 19 Comparison of deterministic, stochastic with the measured values of hydraulic head distribution along x-section of south Buffalo flood plain well and Yow 2 well

As the topography of the surface, between the exit point of Buffalo Creek and the observation well at Gibsonville is flat, constant slope 0.055 percent was estimated using ArcGIS horizontal distance and surface elevation differences. The gradient of hydraulic head is also assumed to be parallel to ground surface slope. Average simulated hydraulic head at exit point of Buffalo Creek is 194.3351 m (amsl) Figure 13 and Figure 16. Annual average groundwater level at Gibsonville monitoring well is 189.8 m (amsl), *Figure 2*. This comes out to be about 0.0476 percent hydraulic head gradient that is in agreement with ground surface slope. Moreover, because the surrogate elevation represented for each cell (200 x 200 m) is average, this variation was considered acceptable. Another output result by MODFLOW is the annual volumetric water budget balance, (input – output). This percentage difference is nearly 0 %, indicating good result. Volumetric water budget output by MODFLOW is also compared and verified with the separated (base flow separation model) and calculated value of base flow.

Groundwater table elevations, calculated on both deterministic and stochastic approaches were also compared. Figure 17 shows the difference of groundwater table depth calculated in both approaches. The variation ranges from a maximum average of five meters starting from relatively high plateau regions towards the steep slope to zero in flat slope regions. This value was considered acceptable because more than seventy percent of grids' water table elevation differences are less than 2 m.

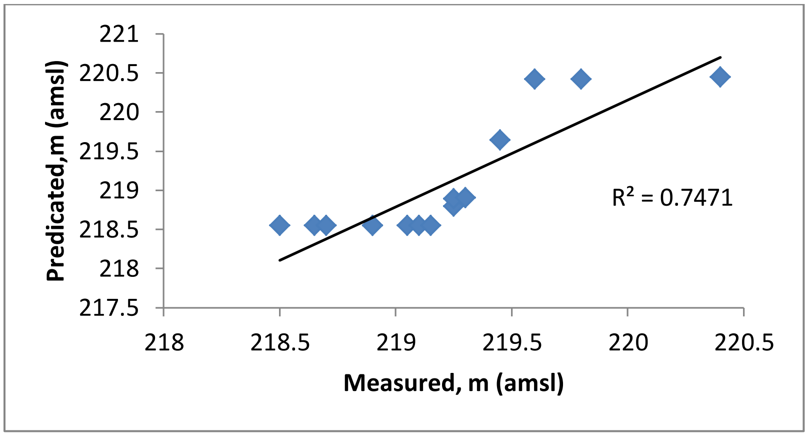
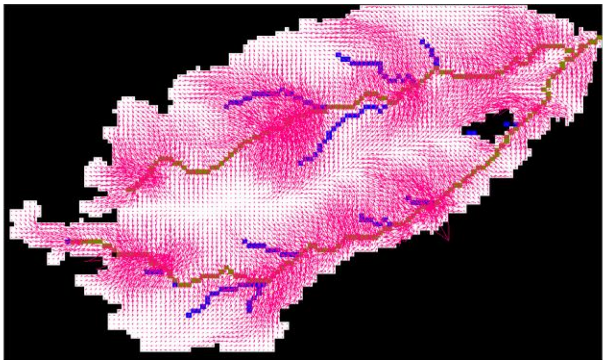
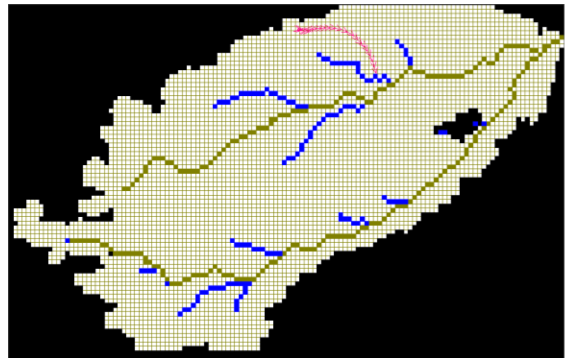


Figure 20 Correlation between measured and model predicted groundwater level

4.2.4 MODPATH. Particle travel time, path line and velocity vector are main outputs of MODPATH. The output file contains the starting coordinate of a particle, the coordinates at every point where it enters a new cell and its final predefined exit coordinate (constant head cells or out of the watershed boundary). For the eight sets of horizontal hydraulic conductivity distribution, the average velocity was calculated, 10^{-7} m/sec. (about 0.9 cm/day). This value is within the range of field and laboratory test results. The length of the vector indicates the relative magnitude of groundwater velocity for that particular cell Figure 21a. In areas where velocity vector magnitudes are large MODPATH assumes potential groundwater flow paths. Travel time and path line analysis was conducted for one of such paths, Figure 21b. Results of four out of six horizontal hydraulic conductivity sets (sets having no dry cell along this particular route) showed average travel time of about 260 years for a particle to reach a pre-defined exit, Figure 22.



(a)



(b)

Figure 21 MODPATH outputs; a) sample velocity vector distribution, b) particle tracking sample from one of potential groundwater flow path (column 67 row 6)

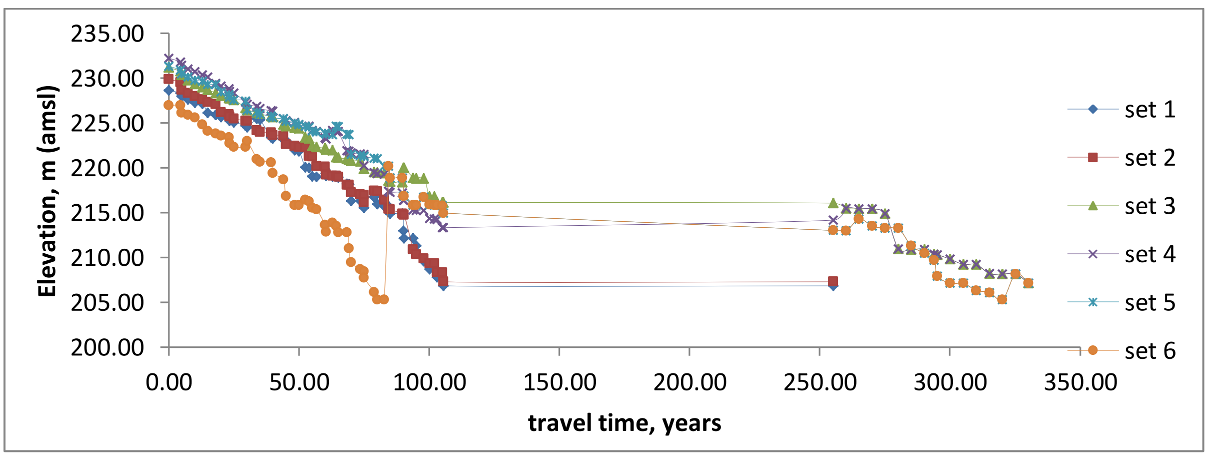


Figure 22 MODPATH output travel time analysis from six runs of different sets (same source location, column 67 row 6) of hydraulic conductivity distribution

South Buffalo wetland is also one of the areas where high velocity vectors were observed. Simulation of groundwater depth profile in the wetland region is at shallower depth as indicated in Figure 23. Any future activity regarding groundwater, either for public consumption or alleviation measures to improve its quality, the forward and backward tracking methods of MODPATH can be more utilized to delineate the capture zone of a well.

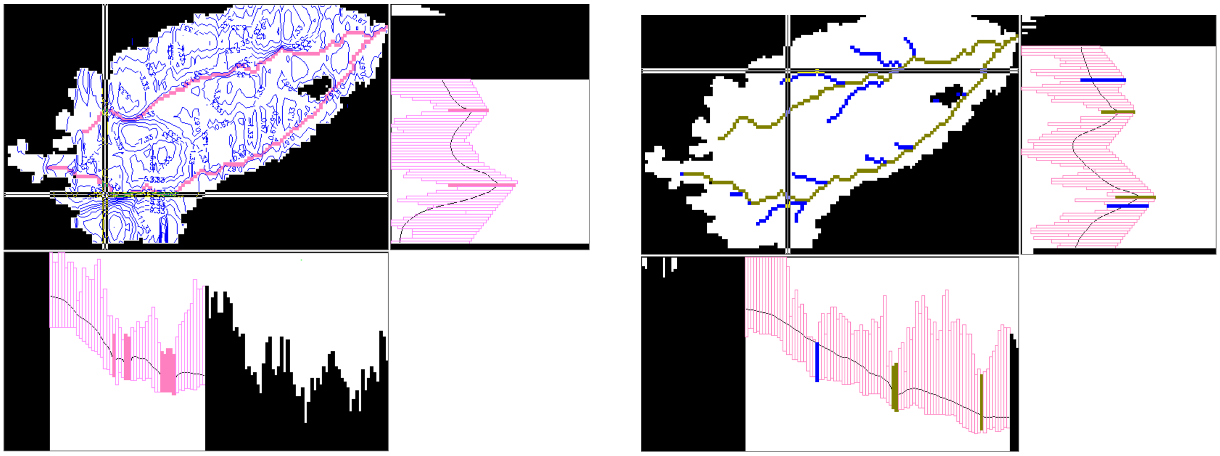


Figure 23 Groundwater elevations along x-section of south Buffalo wetland

4.2.5 MT3D. Continuous discharge from industries and underground storage tanks, and spill from sewerage lines are main sources of groundwater contaminant sources. High flows produced by industries and even homes leaking to sewers… is largely beyond the control of operators of the [sewage treatment] plant makes them susceptible to process upset that can result in discharging constituents beyond the amount permitted by the regulating authorities (the City of Greensboro, 2010). Similarly; the city reported that eight in 2010, four in 2012 and six in 2013 sewage spills from collection system exceeding 1,000 gallons. A total of seventy seven sewer overflows were reported in 2013. Heavy metals are among the most harmful of the elemental pollutants. The city of Greensboro, (2011) reported that; lead (Pb), cadmium (Cd), copper (Cu), and zinc (Zn) are heavy metals associated with industrial discharges and also the brake-pads on cars also contain some of these metals. Brake-pad discharges run off from roads into city streams.

Four locations within the watershed boundary targeting North Buffalo sub-watershed, South Buffalo sub-watershed, both sub-watersheds divide line and near T.Z. Osborn treatment plant were considered for transport modeling. Modeling is performed for two scenarios; continuous source and spill. An initial concentration required by MT3D is defined as 500 mg/L for the first scenario and 5,000 mg/L for spillage were assumed. These amounts were assumed to be the average actual concentration of discharge rate released by industries from the city and the frequent system failure happened by the sewerage system.

The solution scheme used, as discussed in (section 3.6.1) was the hybrid method of characteristic (HMOC). For a particle tracking algorithm, because of the larger tracking time and computational effort required, the fourth order Runge-Kutta and hybrid first order Euler method was used. In MT3D, no flow or dry cells are automatically converted into inactive concentration cells (Chiang, 1996). MT3D generates transport records in ASCII format that can be used for further analysis. For each MT3D run, hydraulic head distribution and velocity vectors are read from MODFLOW and MODPATH outputs, respectively.

For continuous source discharge, the contour plot Figure 24 through Figure 24 2 and the three dimensional view Figure 25 through 25 2 showed that the contaminant plume in flat slope areas like South Buffalo wetland was not propagated to wide area even after one hundred years except in one scenario out the five. Moreover, the plume had never reached the predefined exit (constant head channel or out of the watershed boundary) over a hundred year time.

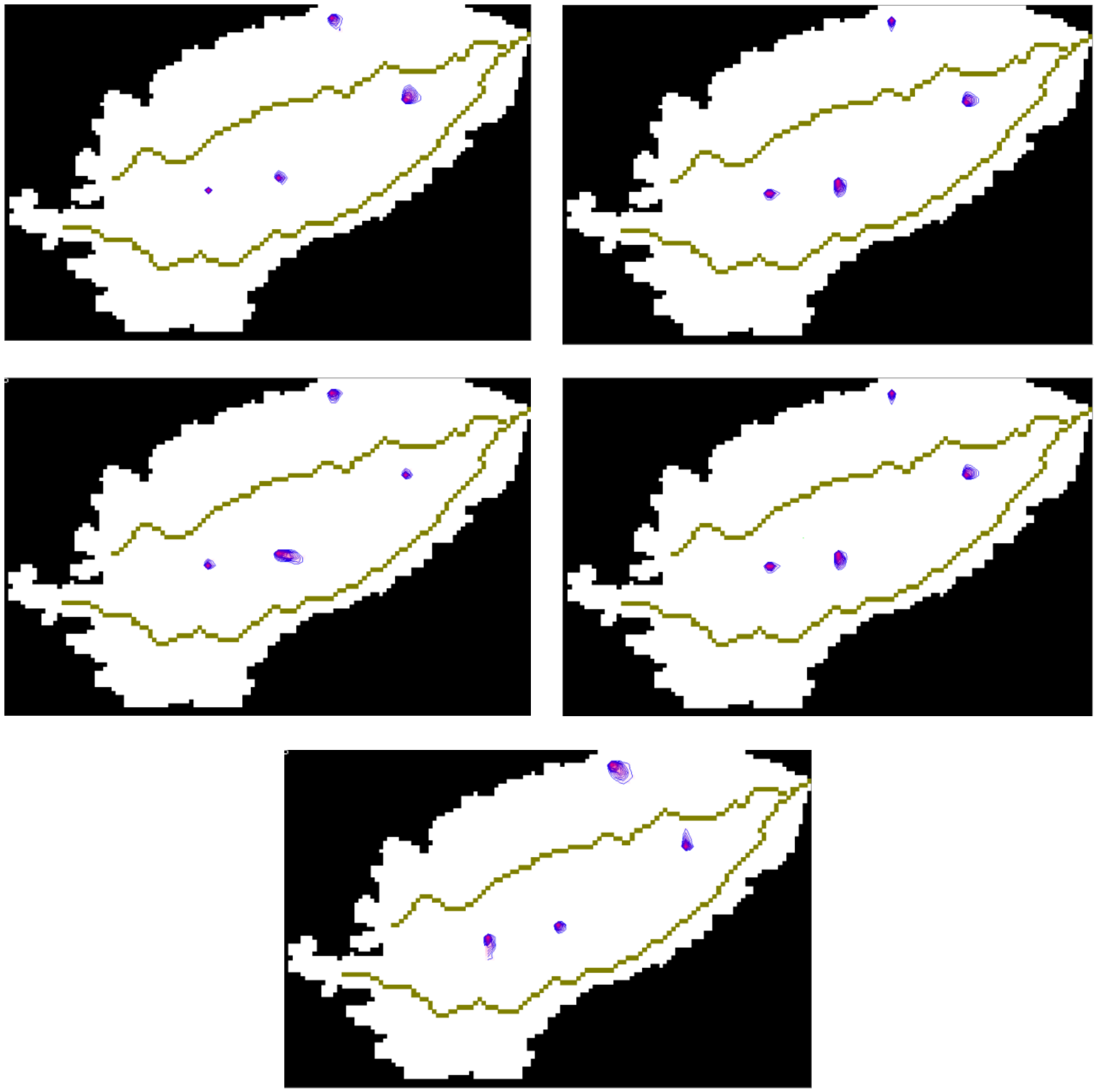


Figure 24 Contour map of continuous source contaminant plume extent for five sets of statistical distributed horizontal hydraulic conductivity values; after ten years

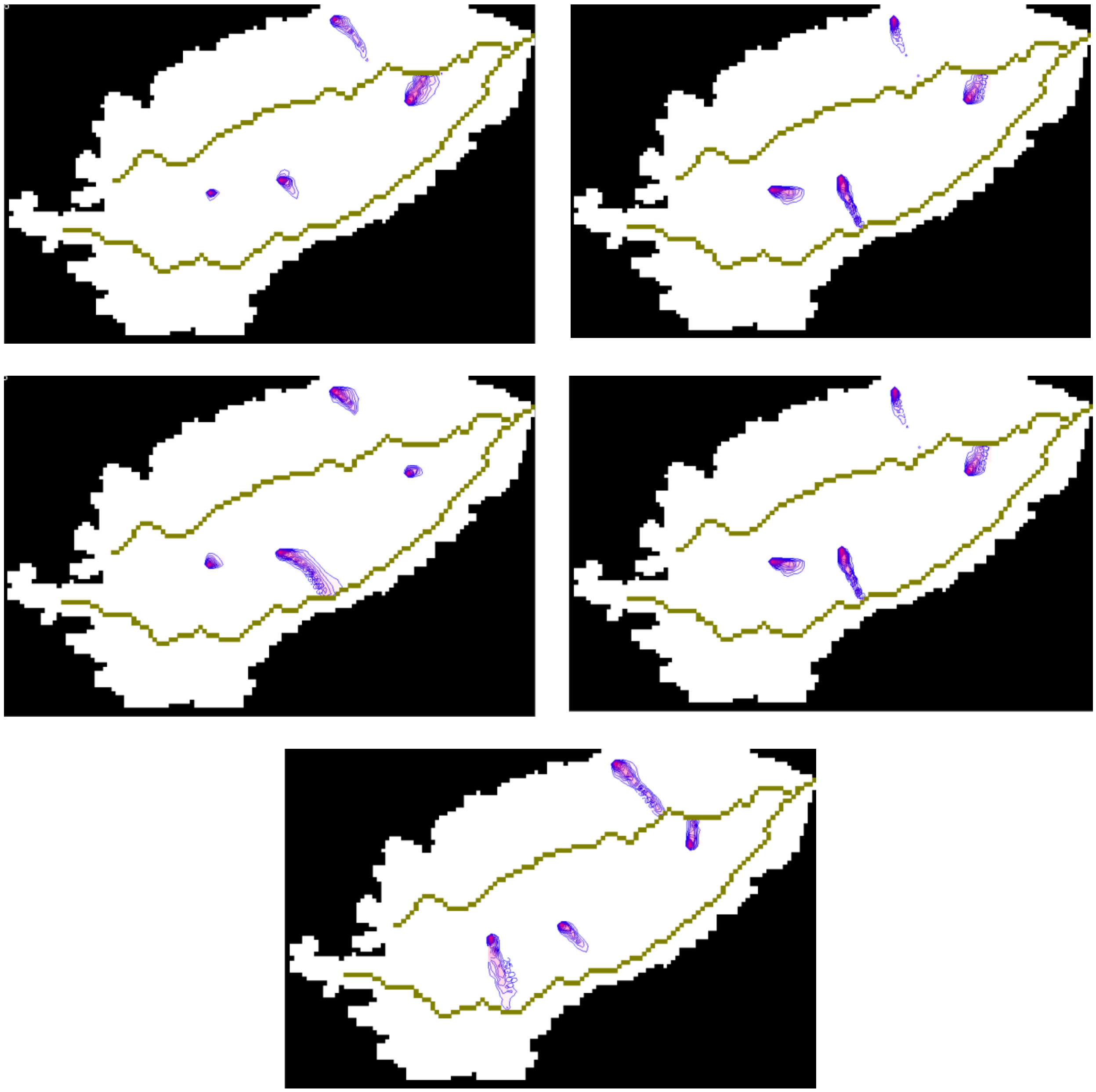


Figure 24 1 Contour map of continuous source contaminant plume extent for five sets of statistical distributed horizontal hydraulic conductivity values; after fifty years

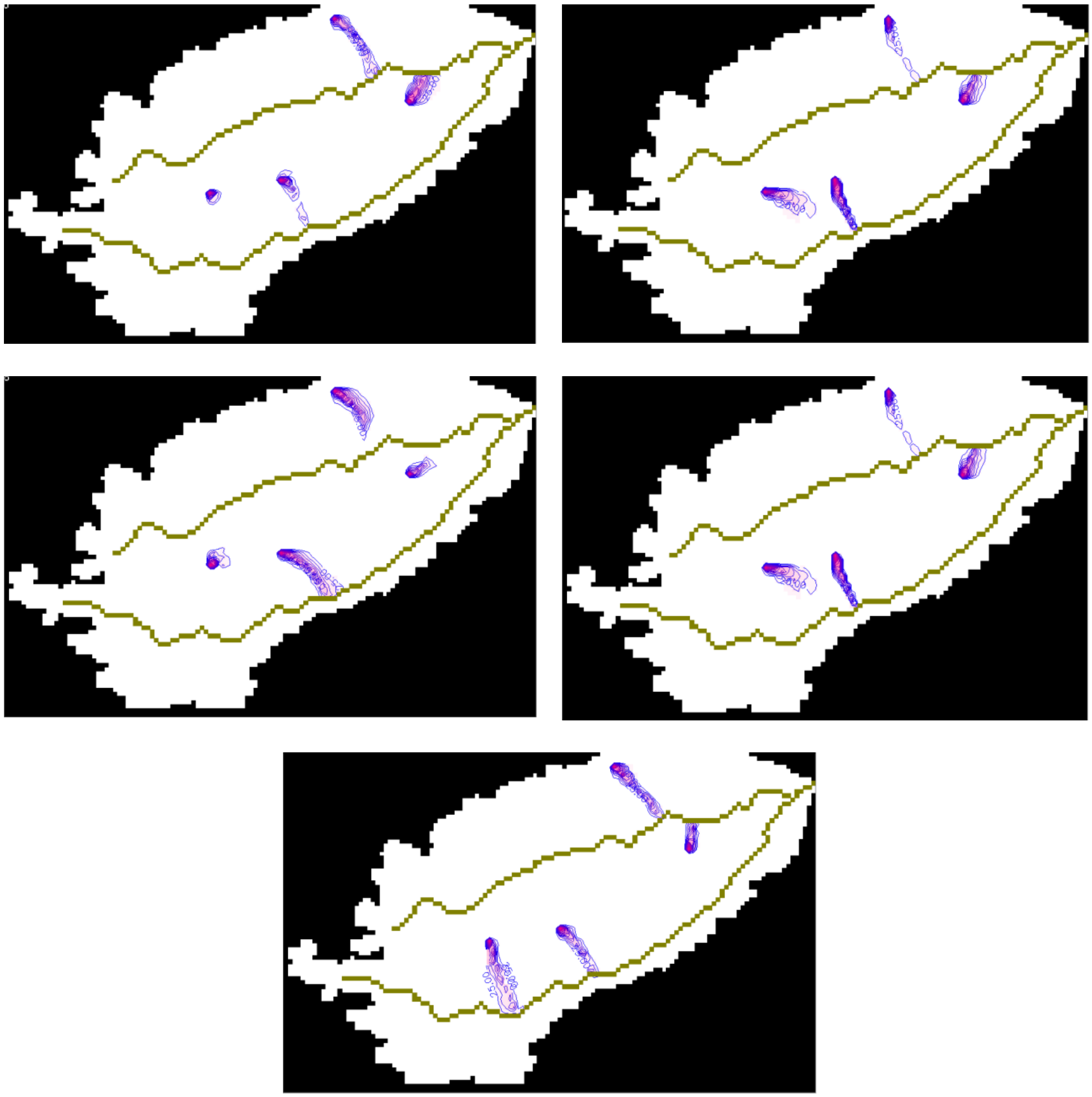
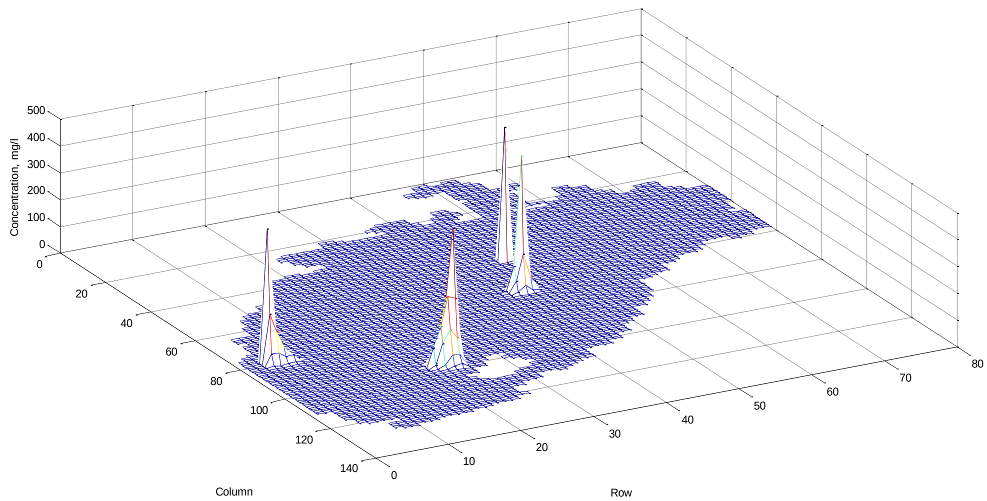
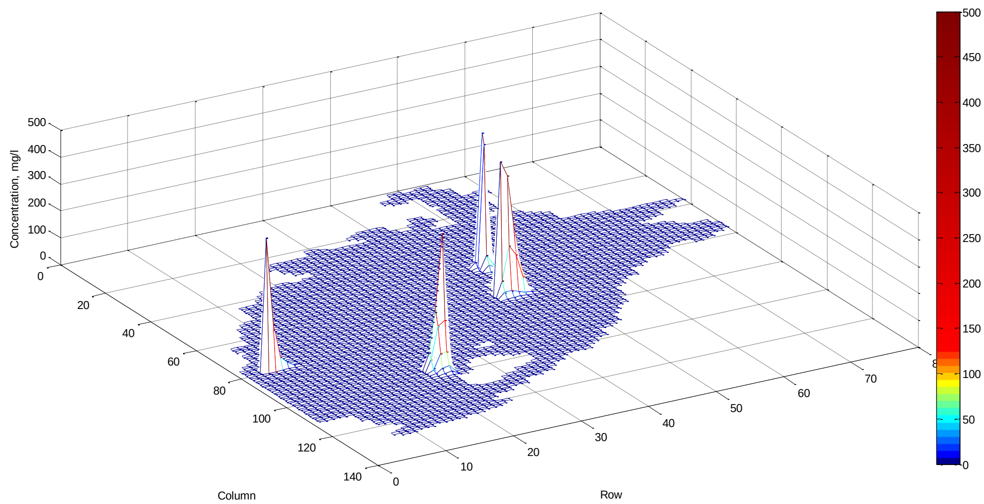


Figure 24 2 Contour map of continuous source contaminant plume extent for five sets of statistical distributed horizontal hydraulic conductivity values; after one hundred years

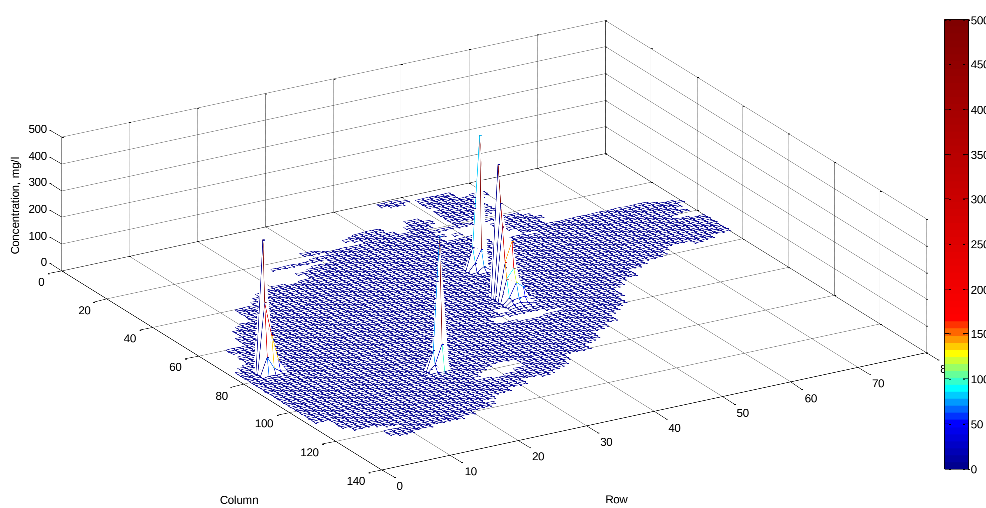
We also observed similar results for the spilled contaminant case. In these regions of the watershed (flat slope), analysis of results for another hundred years period showed that the plume propagation is nil, *Figure 26* and Figure 27. The spilled contaminant concentration in the flat parts of the watershed reduces to only to about 40 percent while the reduction is as high as 88 percent in other locations after 10 years of spill. After one hundred years, all the contaminants gone in some areas while there are still as high as 600 mg/L in flat regions of the watershed. This indicates that the use of groundwater from these regions is not safe due to its high concentration rate of solute. This influence also holds true for plants depending upon contaminant type released in sub-region under consideration. Any remedial measures around the wetland need further study, particularly against environmental impact potential.



Concentration, mg/l
0
100
200
300
400
500
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
80



Concentration, mg/l
0
100
200
300
400
500
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
0
50
100
150
200
250
300
350
400
450
500



Concentration, mg/l
0
100
200
300
400
500
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
0
50
100
150
200
250
300
350
400
450
500

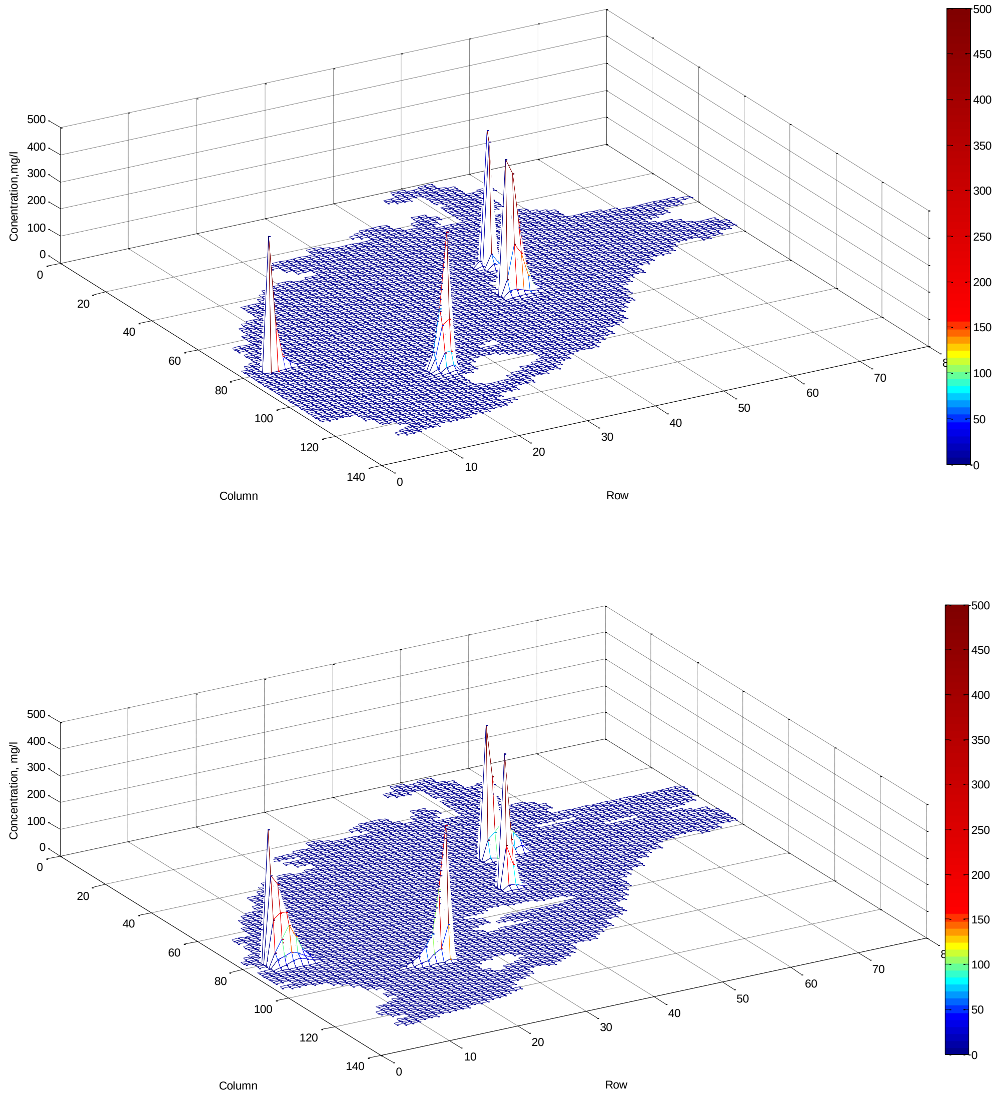
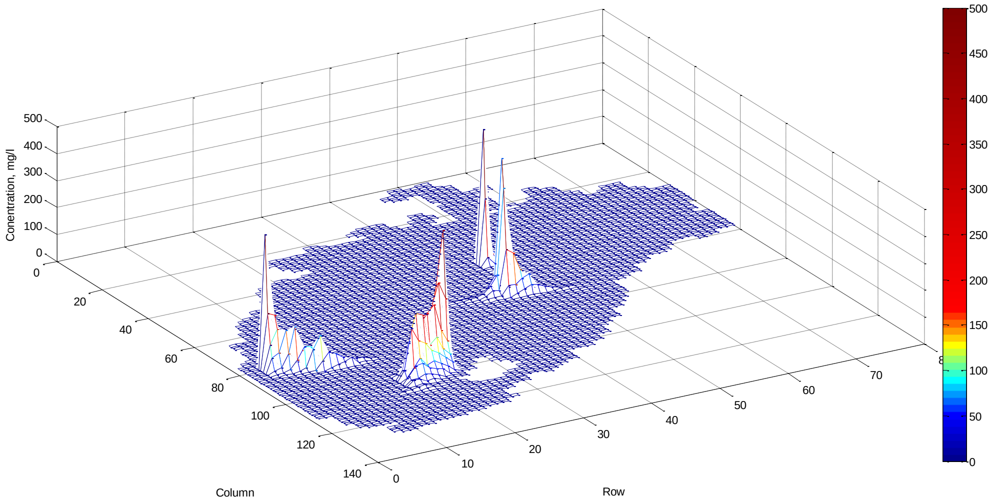
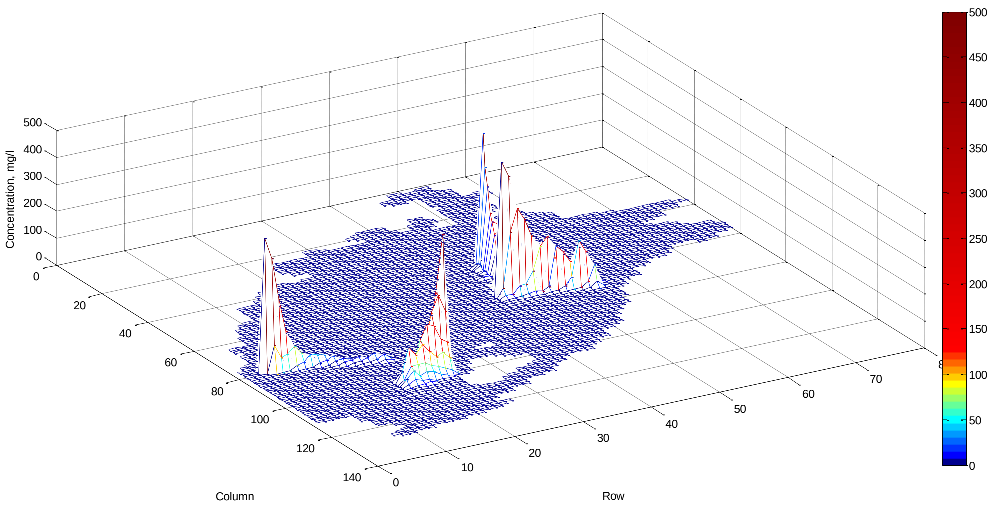
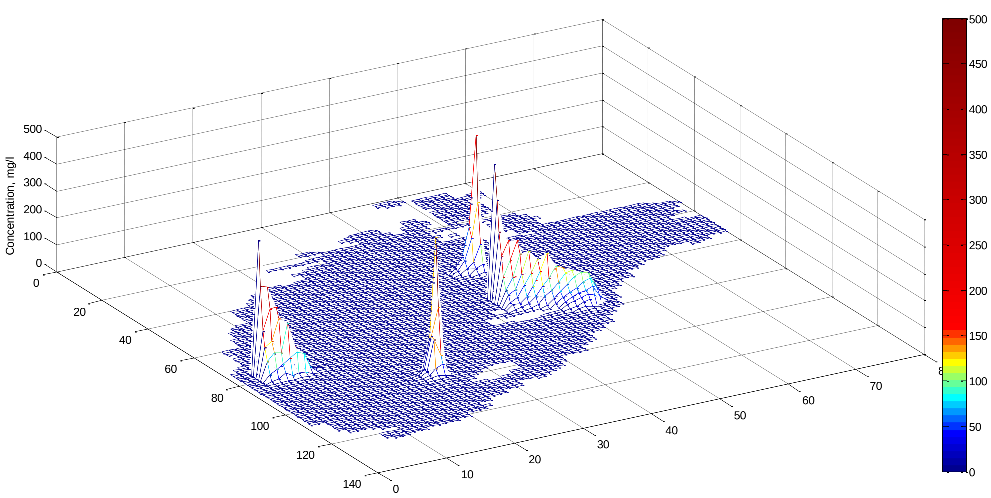


Figure 25 Three dimensional view of continuous source contaminant plum; after ten years


Conentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
500
450
400
350
300
250
200
150
100
50
0


Concentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
500
450
400
350
300
250
200
150
100
50
0


Concentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
0
10
20
30
40
50
60
70
500
450
400
350
300
250
200
150
100
50
0

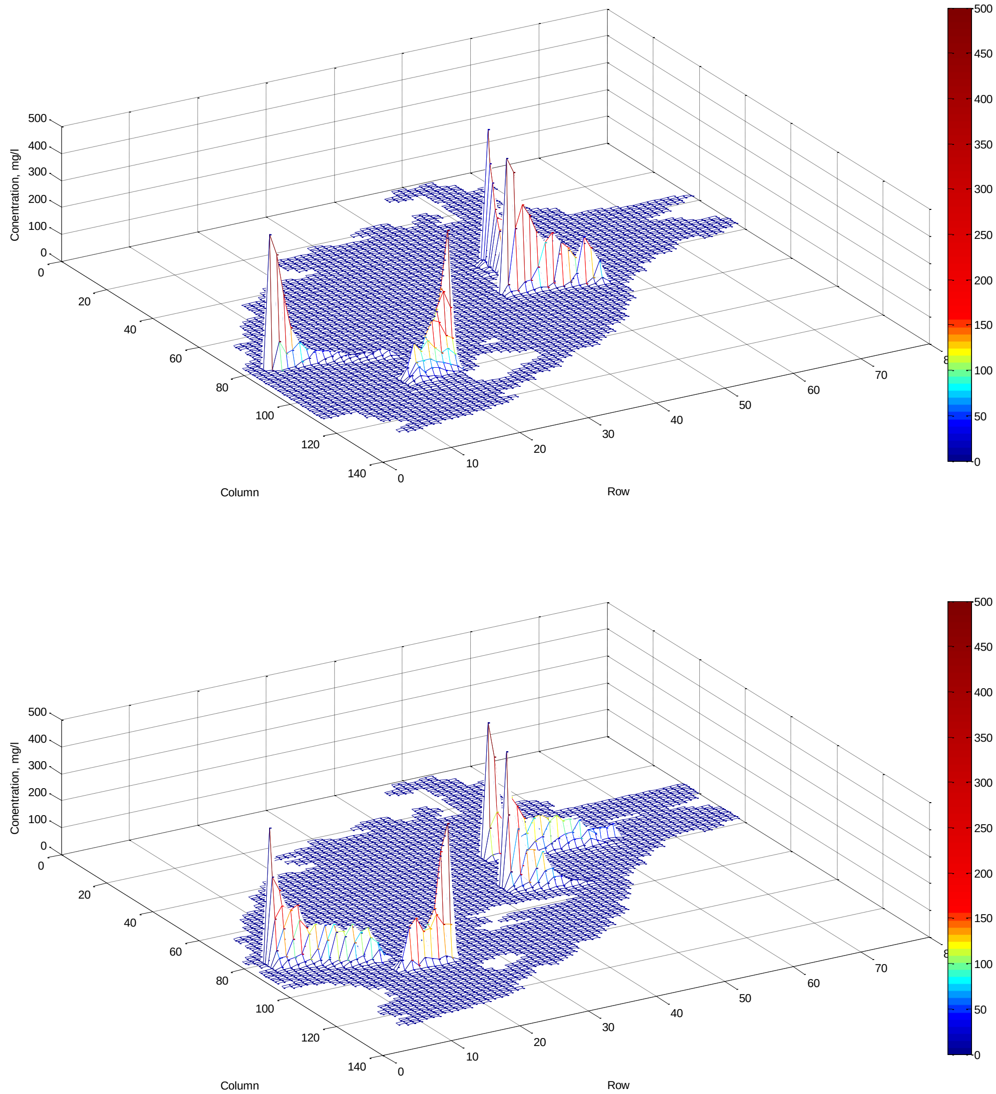
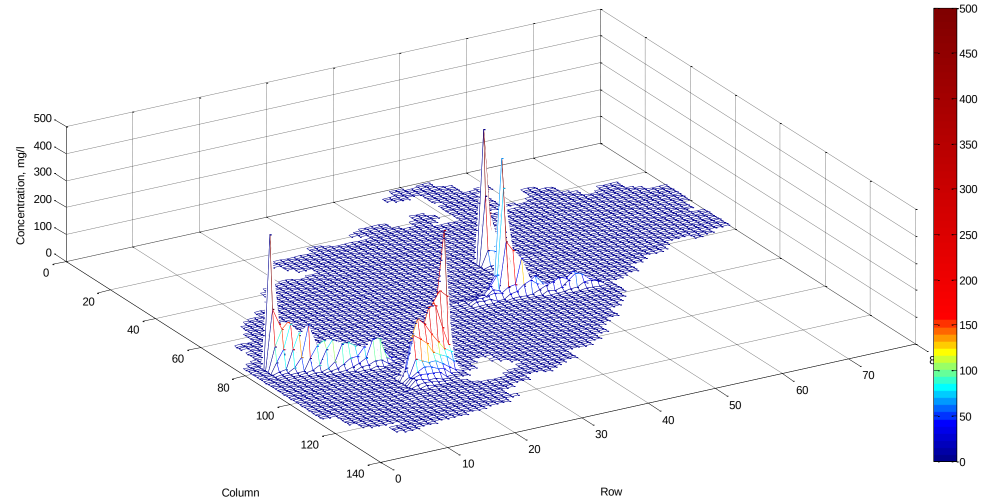
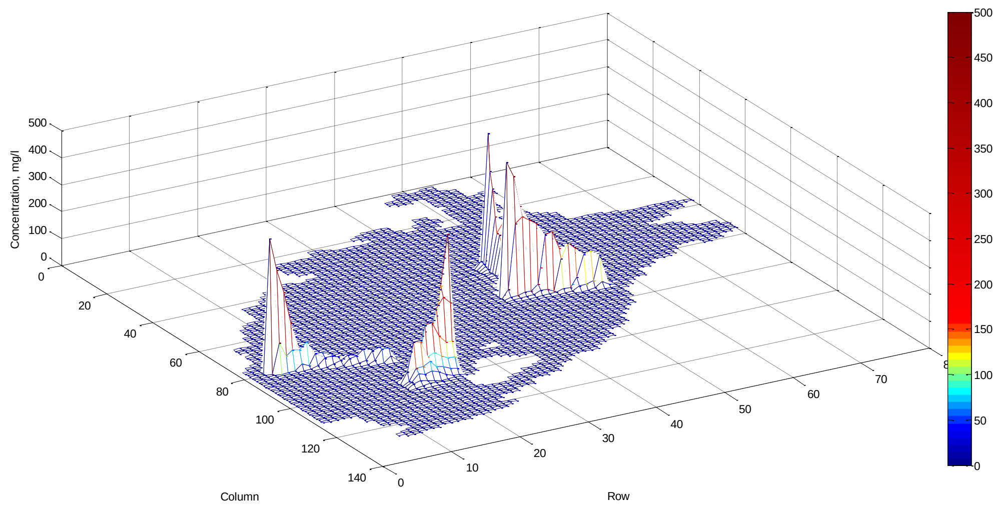
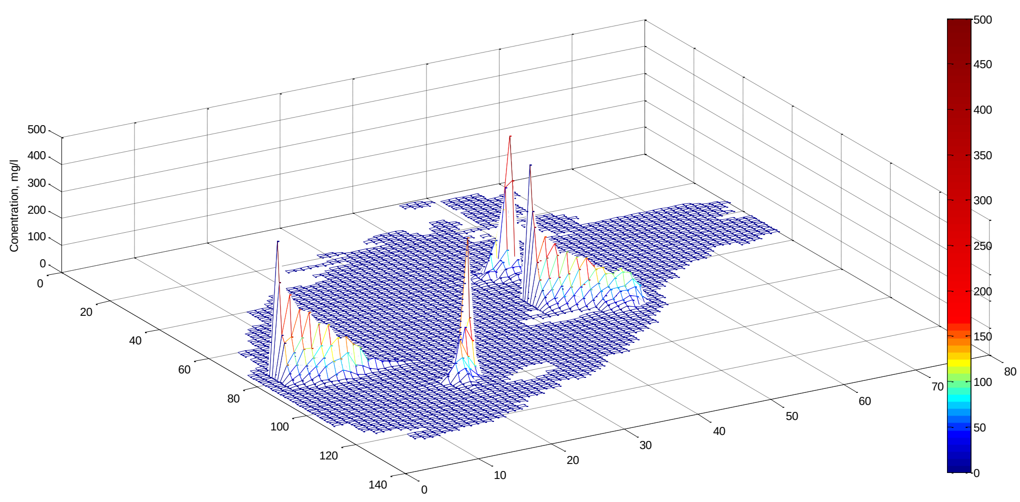


Figure 25 1 Three dimensional view of continuous source contaminant plume; after fifty years


Concentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
10
20
30
40
50
60
70
500
450
400
350
300
250
200
150
100
50
0


Concentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
10
20
30
40
50
60
70
500
450
400
350
300
250
200
150
100
50
0


Conentration, mg/l
500
400
300
200
100
0
Column
0
20
40
60
80
100
120
140
Row
10
20
30
40
50
60
70
80
500
450
400
350
300
250
200
150
100
50
0

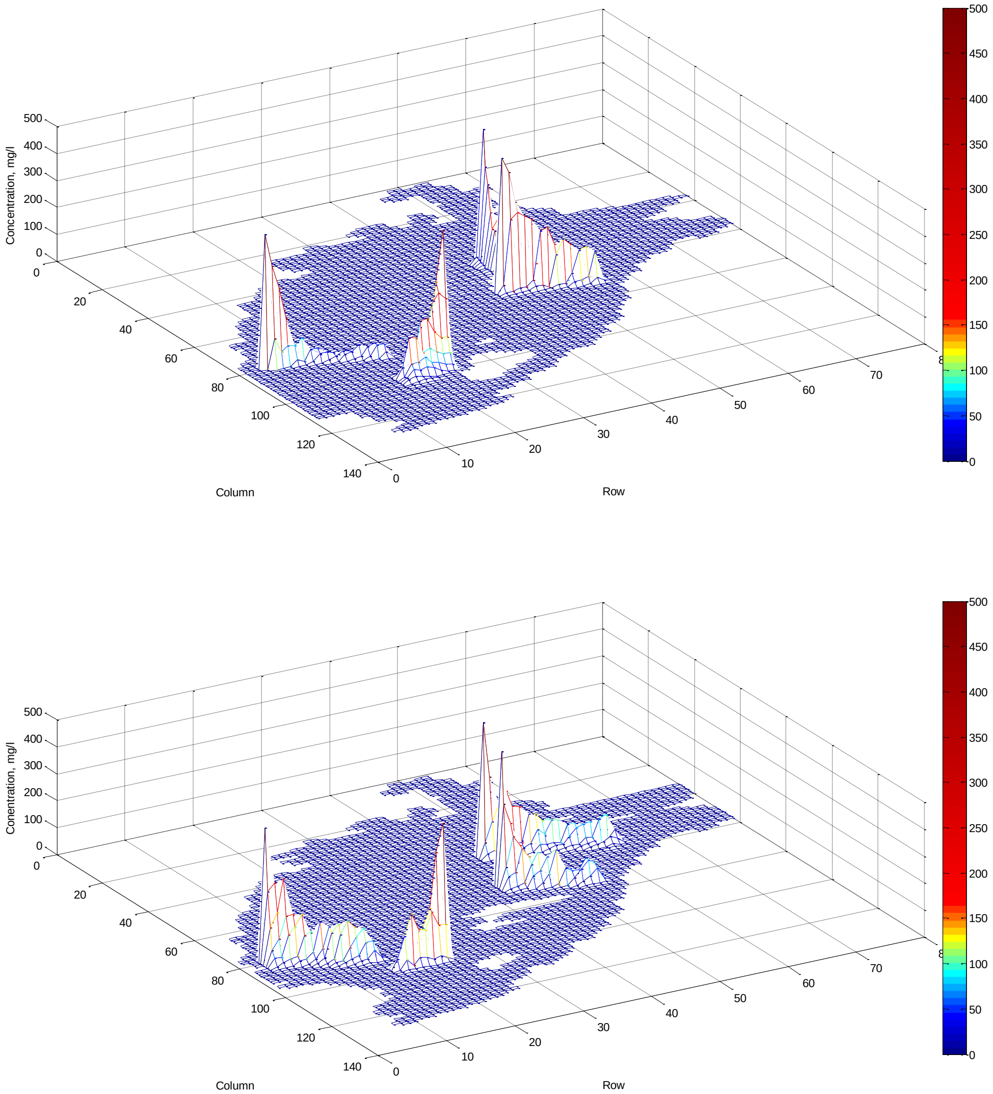
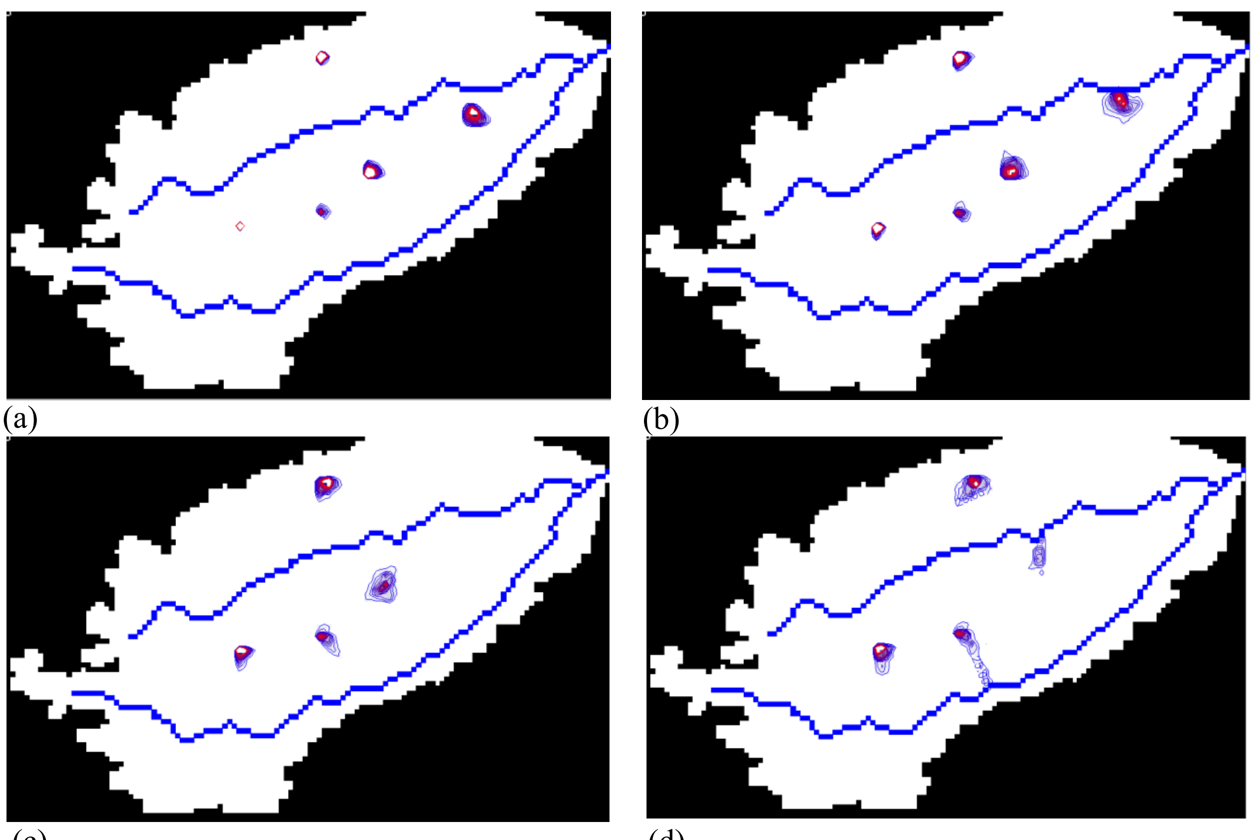


Figure 25 2 Three dimensional view of continuous source contaminant plume; after one hundred years

Table 2

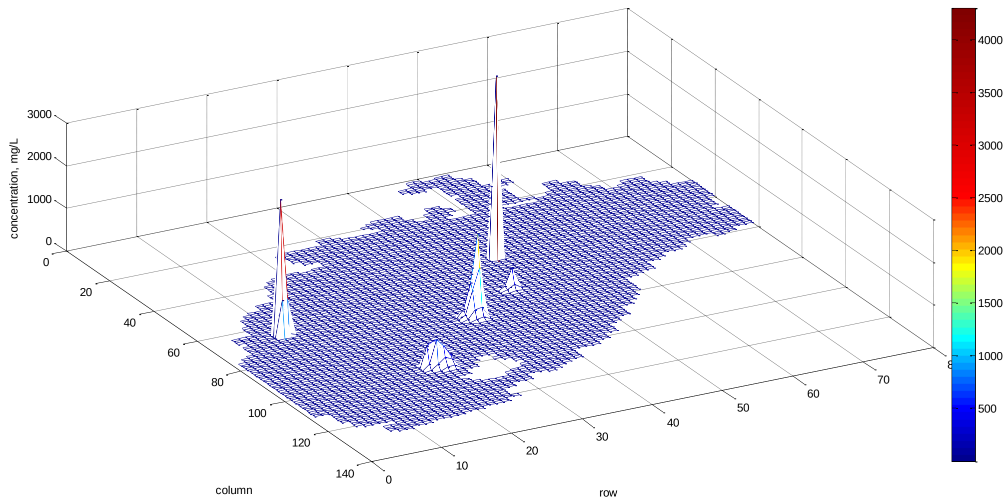
Mass balance comparison for volumetric groundwater flow and contaminant

Hydraulic conductivity	**Volumetric flow**		**Volumetric flow discrepancy (In-out), percent**	**Solute mass discrepancy, (In-out) percent**
	In	**Out**		
Set 1	11056842	11056816	0.000235	4.44
Set 2	12200429	12200294	0.001107	4.32
Set 3	11203907	11203957	-0.000446	1.22
Set 4	11411093	11411177	-0.000736	2.77
Set 5	11694719	11694692	0.000231	-2.31
Set 6	11408088	11407282	0.007065	4.67
Set 7	11423453	11423876	-0.003703	2.69
Deterministic	11318377	11318737	-0.003181	4.21

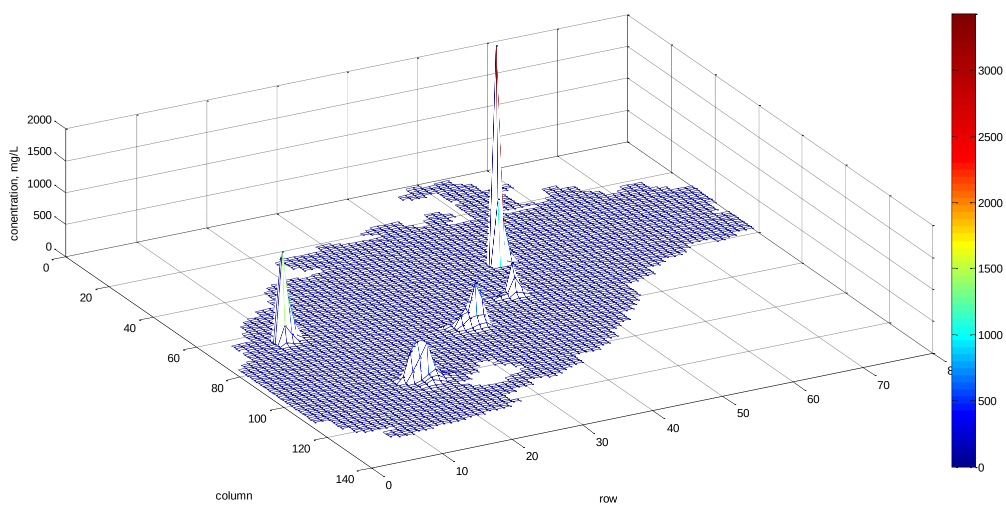


(a) (b) (c) (d)

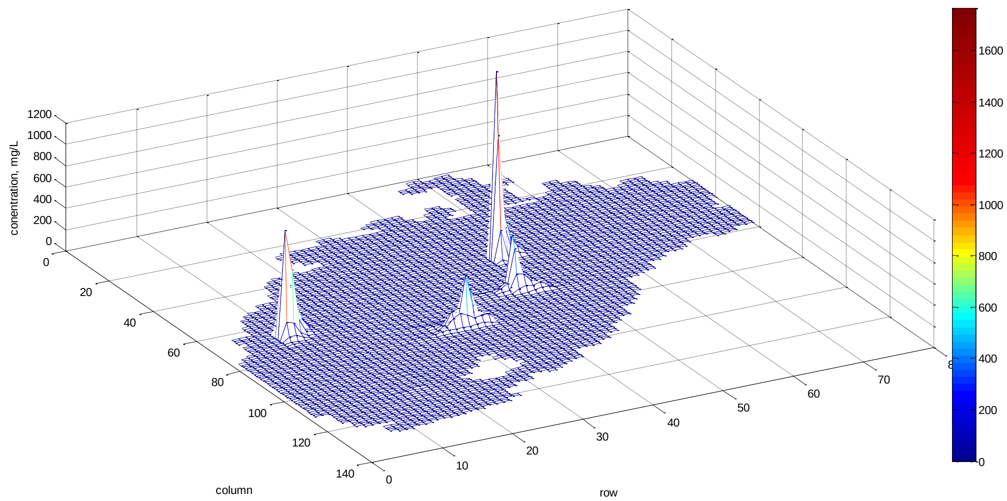
Figure 26 Spilled contaminant plume extent for averaged stochastically distributed horizontal hydraulic conductivity values after; (a) ten years, b) twenty five years, c) fifty years, d) one hundred years



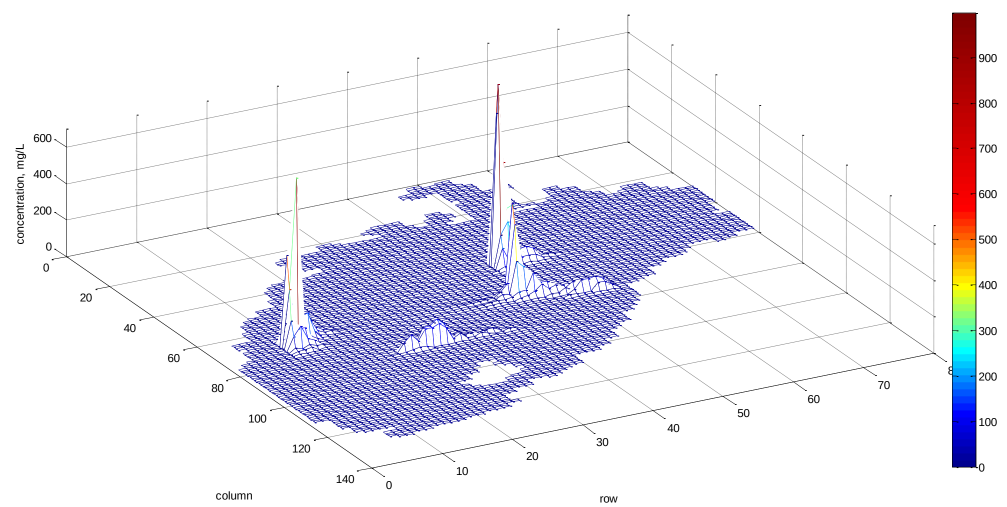
(a)



(b)



(c)



(d)

Figure 27 Spilled contaminant plume extent three dimensional view for averaged stochastically distributed horizontal hydraulic conductivity values after; (a) ten years, b) twenty five years, c) fifty years, d) one hundred years

CHAPTER 5

Conclusion and Recommendations

5.1 Conclusion

It can be concluded that the model was sufficiently accurate except at steep slope locations of South Buffalo sub-watershed. In this sub-region, groundwater flow is dominated by slope factor than aquifers parameters. However, in such regions stochastically distributed parameters can be calibrated and fine-tuned using pump test. The stochastic approach was able to approximate aquifer parameters (in our case horizontal hydraulic conductivity value) better than the deterministic approach. Kriging's method of stochastically distributed hydraulic conductivity values generated lower error than the deterministic approach. An R^2 value of 0.7471 was also considered good match because measured values are data over seasons of the year with expected significant groundwater depth variations over the record period. Major model output results; water budget and solute mass balance for MODFLOW and MT3D respectively were analyzed. Seven of the eight (87 %) and five of the eight (62 %) sets of hydraulic conductivity values ranging from 10^{-3} to 10^{-7} m/sec. were able to generate less error than the deterministic values.

Contaminant plume in flat slope areas like South Buffalo wetland was not propagated to wide area. Moreover, the plume had never reached the predefined exit (constant head channel or out of the watershed boundary) over a hundred year time. We also observed similar results for the spilled contaminant case. In these regions of the watershed, analysis of results for another hundred years period showed that the plume propagation is nil. After one hundred years, all the contaminants gone in some areas while there are still as high as 600 mg/L in flat regions of the watershed. This indicates that the use of groundwater for public consumption from these regions is not safe due to its high concentration rate of solute. This influence also holds true for plants depending upon contaminant type released in sub-region under consideration. In general, groundwater water quality is getting worse through time, particularly from continuous contaminant sources. Due to a constant discharge to ground water, plume's, concentration from these sources keeps on increasing throughout its path. Moreover, this ever increasing contaminant concentration effects cannot be observed shortly, unless monitoring wells introduced throughout the watershed.

Any remedial measures around the wetland need further study, particularly against environmental impact potential. Besides its high discharge amount (about 80 % of the total flow), discharge released from the treatment plant was appropriately considered and introduced to the natural flow system of buffalo basin (a constant head discharge) without altering aquifer parameters. In our assumptions and modeling, source of groundwater was only from areal recharging, part of rainfall infiltrated. However; model results analysis showed that out of the total annual base flow, about 2.97 percent is contributed by stream through aquifer-stream exchange. This also indicates the existence of flow exchange between groundwater and impaired streams, South and North Buffalo affecting groundwater quality too. The exchange rate is expected to be higher when groundwater is getting depleted in extended dry seasons.

5.2 Recommendation

The effects of groundwater quality deterioration take decades and centuries to be visible. Moreover it is difficult or impossible to rehabilitate once its quality gets worsen. Timely monitoring and controlling by respective agencies of major contaminant sources against their discharge release helps future possible multi-dimensional environmental problems. The presence of sufficient monitoring wells across the watershed enhances effective monitoring of water quality and quantity too. This same result can help to integrate and include similar geological formations around regolith of the piedmont and further. For that North Carolina Agricultural and Technical University can take a leading role and work with collaborative relevant organizations such as USGS, NCDWR, so that the watershed can be used as research site for groundwater flow and solute transport in future environmental remedial measures.

References

Abu-EL Sha'r, Y. W. & Hatamleh, I. R., 2007. Using MODFLOW and MT3D groundwater flow and transport model as a management tool for the Azraq groundwater system. *Journal of civil engineering,* 1 (2), 153-172.

Anderson, P. M. & Woessner, W. W., 1992. *Applied groundwater modeling: Simulation of flow and advective transport.* San Diego, USA: Academic press Inc.

Arnold, J. G. & Allen, P. M., 1999. Validation of Automated Methods for Estimating Baseflow and Groundwater Recharge from Stream Flow Records. *Journal of American Water Resources Association,* 35, 411-424.

Bear, J., 1979. *Hydraulics of groundwater*. New York, USA: McGraw-Hill International Book Co.

BPA Environmental and Engineering Inc., 1996. In-situ hydraulic conductivity testing, White Street Landfill, Greensboro, NC. www.greensboro-nc.gov/modules/showdocument.aspx?documented (accessed 6.15.2013)

Boulton, A. J., 2007. Hyporheic rehabilitation in rivers: restoring vertical connectivity. *Freshwater Biology,* 52, 632–650.

Chiang, W. H., 2005. *3D Groundwater Modeling with PMWIN: A Simulation system for modeling groundwater flow and pollution,* (2nd ed.), Lake Forest, CA: Springer.

Chiang, W. H., & Kinzelbatch, W., 1996. Processing MODFLOW: A simulation system for modeling groundwater flow and pollution. *www.pmwin.net/pmwin5.htm* (accessed 7.22.2013)

City of Greensboro, 2011. Sewage Collection and Reclamation Plant: City of Greensboro Open-File- Report. *www.greensboro-nc.gov/Modules/ShowDocument.aspx?documentID(accessed 9.2.2013)*

City of Greensboro, 2010. Water Supply Master Plan 2009: City of Greensboro. Open-File-Report.

Cobel, W. R., Giese, L. G. & Eimers, L. J., 1989. North Carolina Groundwater resources. Open-File-Report, National Water Summary North-Carolina 329. *www.ncwater.org/...and...water/.../NC_Ground_Water_Resources.pd* (accessed 2.4.2013)

Criddle, W.D., 1958. Methods of computing the consumptive use of water: *Journal of the Irrigation and Drainage Division, Proceedings of the American Society of Civil Engineers,* 84, (IR 1), 1-27

Daniel, C. C. & Harned, A. D., 1998. Ground-Water Recharge to and Storage in the

Regolith-Fractured Crystalline Rock Aquifer System, Guilford County, North Carolina. *United States Geological Survey*, Open-File-Report 97-4140.

Daniel, C. C., III, & Sharpless, N.B., 1983. Groundwater supply potential and procedures for well-site selection in the Upper Cape Fear River Basin, North Carolina. *North Carolina Department of Natural Resources and Community Development and U.S Water Resources Council*, 73.

Daniel, C. C., III, White, K. R., & Stole, A. P., 1989. Groundwater in the Piedmont of the Eastern United States. *Proceedings of a conference* October 16-18, 1989, Charlotte, North Carolina.

Davenport, S. M., 1989. Water Quality in Reedy Fork and Buffalo Creek Basins in the Greensboro Area, North Carolina, 1986-87. *Water Resources Investigations Report. U.S. Department of the Interior, Geological Survey.*

David, P., 1988. Documentation of computer programs to compute and display pathlines using results from the U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model: U.S. Geological *Survey,* Open-File Report 89-381.

Doherty, J., 1994. *PEST, Model independent parameter estimation. Watermark numerical computing.* (4th ed.) USA: EPA.

ESRI, ArcGIS online Resources.

Frankworth, K.R., & Thompson, S.E., 1982. Pan Evaporation Data for North Carolina. *NOAA Technical Report NWS* 34, Open-File-Report.

Floyd, O. E. & Peace, R. R., 1974. An appraisal of groundwater resources of the Upper Cape Fear River basin North Carolina: *Groundwater Bulletin number* 20; U.S. Geological Survey and North Carolina Office of Water and Air Resources.

Harbaugh, A.W., Banta, E.R., Hill, M.C., & McDonald, M.G., 2000. MODFLOW-2000, The U.S, Geological Survey Modular Ground-Water Model – User Guide to Modularization concepts and the Ground-water Flow Process: Open-File Report 00-92, 121.

Haro, S. P., Velazquez, M. P., & Albert, C. L., 2011. Stochastic hydro-economic modeling for optimal management of agricultural groundwater nitrate pollution under hydraulic conductivity uncertainty. *Environmental Modelling & Software.* 26, (8), 999-1008.

HDR Engineering, Inc., 1997. The phase II expansion of the White Street sanitary landfills. City of Greensboro, construction permit application, project no. 06770-021-018.

HERA Team, 2007. Guilford County groundwater monitoring network status report. *Department of public health.* Open-File Report.

Hill, C. M., 1990. Preconditioned Conjugate-Gradient 2 (PCG2), a computer program for solving groundwater flow equations. *U.S. Geological Survey, water resources investigation report* 90-4048.

John, C. B., Kevin, J. B., Charles, A. J., & Mary, J. K., 2007. Assessing the economic benefit of groundwater for environmental policy decision. *Journal of the American Water Resources Association,* 32, (2)**,** 279–291.

Kasahara, T. & Hill, R. A., 2008. Modeling the effects of lowland stream restoration projects on stream–subsurface water exchange. *Ecological engineering*, 32, (4), 310–319.

Kenneth, S. C., 1993. Effect of urbanization and season on concentration of five heavy metals in North Buffalo Creek. *The Journal of Elisha Mitchell Scientific Society,* 109, (3), 152-157.

Kopec, & Clay, 1975. Guilford County Groundwater Monitoring. *Department of Public Health*: status report. www.co.guilford.nc.us/gheh_cms/hera/forms/NetworkReport.pdf (accessed 1.26.2013).

Larsson, M., Niemi, A. & Tsang, C. F., 2012. An observed error in PMPATH particle tracking algorithm for MODFLOW in case of varying porosity and a proposed correction. *Computers & Geosciences*, 45, 1–3.

Leonard, F. K., 2011. The secret to successful solute-transport modeling. *Groundwater issue* 49, (2), Groundwater, 144-159.

Lyne, V.D. & M. H., 1979. Stochastic time variable rainfall-runoff modeling. *Hydro and water resource symposium.* Institution of Engineers, Perth, Australia, 89-92.

Matthews, K. Y., 2002. Functional assessment for proposed flood plain storm water treatment wetland. *Graduate class of North Carolina State University, Natural Resources, Hydrology*, Raleigh open File Report.

McDonald, G. M. & Harbaugh, W. A., 1984. A Modular three dimensional finite difference groundwater flow model. *U.S Geological Survey* Open-File-Report 83-875.

Nathan, & McMahon, 1990. Regional estimation of base flow for the conterminous United States by hydrologic landscape regions. *Journal of Hydrology,* 351, 139-153.

Nathan, R. J. & McMahon, T. A., 1990. Evaluation of automated techniques for baseflow and recession analysis. *Water Resources Res.*, 26, 1465-1473.

North Carolina Department of Environment and Natural Resources, 1999. Basin wide assessment report Cape Fear River Basin. *North Carolina Department of Environment and Natural Resources, Division of Water Quality,* Open-File-Report.

Peter, F. A., 1993. A manual of instructional problems for the U.S.G.S. MODFLOW model. *United States Environmental Protection Agency,* EPA/600/R-93/10, Open-File-Report.

Pfaender, K. F., Shuman, S. M., Dempsey, H. & Harden, C. W., 1977. Monitoring heavy metals and pesticides in the Cape Fear River Basin of North Carolina. *Department of Environmental Sciences and Engineering, School of Public Health, University of North Carolina,* Chapel Hill, Open-File-Report.

Pollock, D.W., 1994. User's Guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow Model. *U.S. Geological Survey,* Open-File Report 94-464.

Price, K., Jackson, C. R., & Parker, J. A., 2010. Variation of surficial soil hydraulic properties across land uses in the southern Blue Ridge Mountains, North Carolina, USA. *Journal of Hydrology*, 383, (3–4), 256–268.

Prudic, E. D., 1989. Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model. *U.S. Geological Survey,* Open-File Report 88-729.

Prudic, E. D., Konikow, F. L., & Banta, R. E., 2004. A New Stream Flow-Routing (SFR1) Package to Simulate Stream- Aquifer Interaction with MODFLOW -2000. *U.S. Geological Survey,* Open File-Report 2004-1042.

Rahmawati, N., Vuillaume, F. J., & Purnama, S. L., 2013. Salt intrusion in coastal and lowland areas of Semarang City. *Journal of hydrology,* 494, 146–159.

Rivett, O., Michael, E. A., Paul, & Mackay, R., 2011. Urban groundwater base flow influence up on inorganic River-Water quality: The River Tame Headwaters Catchment in the City of Birmingham, United Kingdom. *Journal of Hydrology*, 400, (1–2), 206–222.

Ruskauff, J. G., 1998. Guide to using Stochastic MODFLOW for Monte Carlo Simulation. http://pages.geo.wvu.edu/~donovan/ftp/stochdoc.pdf (accessed 06.09.2013).

Schulz, E.F., 1973. *Problems in applied hydrology,* (7 th ed.): Fort Collins, Colorado, USA: Water Resources Publications.

Sykes, J. F., Randall, J. E., & Normani, S. D., 2006. The analysis of seasonally varying flow in a crystalline rock watershed using an integrated surface water and groundwater model. *American Geophysical Union,* Open-File-Report.

Terziotti, S., Schrader, P. T., & Treece, M. W., 1990. *Estimated water use by county in North Carolina,* (2nd ed.), Raleigh, N.C: *U.S.* Geological Survey.

U.S. Geological Survey, 1997. Modeling groundwater flow with MODFLOW and related programs. Fact Sheet FS-121-97.

U.S. Geological Survey, Page last modified: January 24, 2012. Shuttle Radar Topography Mission. Long term Open-File-Archive.

U.S. Environmental Protection Agency, 2008. Groundwater rule source assessment. Open-File-Report 815-R-07-023.

U.S. Environmental Protection Agency, 1991. Getting up to speed groundwater contamination. *www.epa.gov/region1/students/pdfs/gwc1.pdf* (accessed 01.15.2014).

Winner, M.D.,Jr., Simmons, C.E., 1977. Hydrology of the creeping swamp watershed, North Carolina, with reference to potential effects of stream channelization: *U.S. Geological Survey Water Resources Investigation Report* 77-26, 54 p.

Winter, C. T., & Harvey, W. J., 1998. Groundwater and Surface Water a single source. U,S Geological Survey Circular 1139.

Winter, C. T., Rosenberry, O. D., & LaBaugh, W. J., 2003. Where does the groundwater in small watersheds comes from? *Groundwater.* 41, (7), 989-1000.

Zheng, C., 1990. MT3D, A Modular 3-D transport model for simulation of advection, dispersion and chemical reaction of contaminants in groundwater system. *Report to the United States Environmental Protection Agency,* 170 pp.