A DISSERTATION ON

QGIS-BASED ASSESSMENT OF GROUNDWATER CONTAMINATION IN MATHURA, UP

SUBMITTED IN PARTIAL FULFILLMENT FOR THE AWARD OF DEGREE OF

MASTER OF TECHNOLOGY IN ENVIRONMENTAL ENGINEERING

SUBMITTED BY:

MANOJ KUMAR (2K19/ENE/02)

UNDER THE SUPERVISION OF Mr. ANUNAY A GOUR



DEPARTMENT OF ENVIRONMENTAL ENGINEERING DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of engineering) Bawana Road, Delhi-110042

July 2021

DEPARTMENT OF ENVIRONMENTAL ENGINEERING DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of engineering) Bawana Road, Delhi-110042

CERTIFICATE

This is to certify that the project report entitled "QGIS-BASED ASSESSMENT OF GROUNDWATER CONTAMINATION IN MATHURA, UP" is a report of the major project done in the partial fulfilment of the requirement for the award of the degree of the Master of Technology in Environmental Engineering from Delhi Technological University during the year 2021 under my supervision.

Mr. ANUNAY A. GOUR

Date:

Place:

DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of engineering) Bawana Road, Delhi-110042

CANDIDATE'S DECLARATION

I Manoj Kumar, 2K19/ENE/02 student of M.Tech. Environmental Engineering, hereby declare that the project dissertation entitled "QGIS-BASED ASSESSMENT OF GROUNDWATER CONTAMINATION IN MATHURA, UP" which is submitted by me to the Department of Environmental Engineering, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Technology is original and not copied from any source without proper acknowledgement. The work has not been submitted in part or full for the award of the degree or diploma in this or any other institute.

MANOJ KUMAR Univ. Roll No.:2K19/ENE/02

Date:

Place:

ACKNOWLEDGEMENT

The dissertation is an important part of the degree of Master of Technology in Environmental Engineering. No research can be accomplished without the guidance of the research supervisor cooperation of faculty members and team. I would like to thank all those who helped me directly or indirectly in getting this task done. It gives me immense pleasure to take this opportunity to thank my guide Mr Anunay A Gour for his enthusiasm, support and guidance that helped me to pursue this research work entitled "QGIS-BASED ASSESSMENT OF GROUNDWATER CONTAMINATION IN MATHURA, UP". Lastly, I would like to thank and salute my parents and almighty God for continuously showering blessings that make me reach up to this level in my career.

-Manoj Kumar

ABSTRACT

This research comprehensively investigates literature about modelling techniques used in groundwater contaminant transport modelling. Modelling of groundwater is a useful way for the management of groundwater resources, also assessing the fate of contaminants and their remediation. Models very conveniently help to study complex real conditions and examine specific phenomena in addition to predicting the future behaviour of any problem. The use of groundwater simulation programming tools such as MODFLOW, MT3DMS, RT3D, FEFLOW, and MODPATH to model multi-directional contamination transport yields accurate results. Movement, storage, and change of solute concentration are largely regulated by groundwater flow gradient. As a result, a precise description of the flow mechanism is very important. If models are not properly constructed and interpreted, they can become complicated and may generate wide errors. Well-defined and clear modelling objectives produce suitable models for efficient error-free modelling processes. The study will assist modellers to clearly define their model objective and select appropriate modelling tools.

This work focuses on groundwater quality investigation using analytic and geographic information system (GIS) to find acceptable groundwater sites for drinking and irrigation in the Mathura district also. The values of physio-chemical parameters of main ions for the 20 sites of water samples collected from the CGWB website were compared to World Health Organization (WHO) and Bureau of Indian Standards (BIS) values. When compared to the WHO and BIS criteria, the results demonstrate that Total Dissolved Solids (TDS), Total Hardness (TH), Mg, F, Electrical Conductivity (EC) and Cl are found to be higher than (>50%) the permitted level. In order to determine potential

groundwater locations for drinking and irrigation, the spatial distribution of several physio-chemical parameters was also plotted in the GIS environment. The resulting integrated water quality map demonstrates that, except for several areas in north-west Mathura and the southern region, the water quality in the Mathura district is mostly unfit for drinking and irrigation.

TABLE OF CONTENTS

| Certificate | |
|-------------|---|
| Candidate's | Declarationiii |
| Acknowledg | ementiv |
| Abstract | |
| Chapter 1. | Introduction |
| 1.1 Nu | merical Models |
| 1.1.1 | Finite Difference Method |
| 1.1.2 | Finite element method |
| Chapter 2. | Literature review |
| 2.1 Mi | gration of Solutes in Groundwater4 |
| 2.1.1 | Governing Equations |
| 2.2 Mo | odelling Approach |
| 2.2.1 | Formulating modelling objectives7 |
| 2.2.2 | Conceptual Model 7 |
| 2.2.3 | Boundary Value Problem |
| 2.2.4 | Selection of modelling software |
| 2.2.5 | Model Design |
| 2.2.6 | Model Calibration |
| 2.2.7 | Model Verification |
| 2.2.8 | Sensitivity Analysis |
| 2.2.9 | Uncertainty Analysis 10 |
| 2.3 Sir | nulator Softwares for Transportation and Ground water flow modelling 10 |
| 2.3.1 | MODFLOW Software (USGS Modular 3-Dimensional Groundwater Flow Mode) 10 |
| 2.3.2 | FEFLOW (finite element subsurface and transport system) |
| 2.3.3 | HST3D (3-D Heat and Solute Transport Model) |
| 2.3.4 | SUTRA (3-D Saturated/Unsaturated Transport Model) |

| 2.3.5 | 5 Use of GIS and Meshfree techniques 1 | 3 |
|------------|--|----|
| Chapter 3. | METHODOLOGY 1 | 5 |
| 3.1 | Steps involved in interpolation 1 | 7 |
| 3.2 | Study Area | 20 |
| 3.3 | Analysis of data | 21 |
| Chapter 4. | RESULTS AND DISCUSSION | 23 |
| 4.1 | Electrical conductivity | 23 |
| 4.2 | Total dissolved solids | 24 |
| 4.3 | Sodium | 25 |
| 4.4 | Calcium | 26 |
| 4.5 | Magnesium | 27 |
| 4.6 | Total Hardness | 27 |
| 4.7 | Nitrate | 28 |
| 4.8 | Sulphate | 29 |
| 4.9 | Bicarbonate | 29 |
| 4.10 | Chloride | 30 |
| 4.11 | рН | 31 |
| 4.12 | Fluoride | 32 |
| 4.13 | Correlation chart | 32 |
| Chapter 5. | Conclusion | 34 |
| Reference | es | 35 |
| Vitae | | 37 |

List of figures

| Figure 1.1 Discretization of space in FDM |
|---|
| Figure 1.2 Discretization of space in FEM |
| Figure 2.1 Modelling process flow chart(Baalousha, 2005) |
| Figure 2.2 Workflow of FEFLOW and MODFLOW (Fouad et al., 2018) 12 |
| Figure 3.1 Add data set into QGIS 17 |
| Figure 3.2 Export data to shapefile |
| Figure 3.3 IDW interpolation |
| Figure 3.4 Change symbology 20 |
| Figure 3.5 Location of study area and sites of groundwater samples in Mathura district India . 21 |
| Figure 4.1 Iso-concentration map showing the spatial distribution of Electrical Conductivity 24 |
| Figure 4.2 Iso-concentration map showing the spatial distribution of Total Dissolved Solids 25 |
| Figure 4.3 Iso-concentration map showing the spatial distribution of Sodium |
| Figure 4.4 Iso-concentration map showing the Spatial distribution of Calcium |
| Figure 4.5 Iso-concentration map showing the spatial distribution of Magnesium |
| Figure 4.6 Iso-concentration map showing the spatial distribution of Total Hardness |
| Figure 4.7 Iso-concentration map showing the spatial distribution of Nitrate |
| Figure 4.8 Iso-concentration map showing the spatial distribution of Sulphate |
| Figure 4.9 Iso-concentration map showing the spatial distribution of Bicarbonates |
| Figure 4.10 Iso-concentration map showing the spatial distribution of Chloride |
| Figure 4.11 Iso-concentration map showing the spatial distribution of pH |
| Figure 4.12 Iso-concentration map showing the spatial distribution of Fluoride |
| Figure 4.13 Correlation chart |

List of tables

| Table 3.1 Descripti | ve statistics | and ran | ge of | parameters | in | groundwater | samples | and | their |
|---------------------|---------------|-----------|-------|------------|----|-------------|---------|-----|-------|
| comparison with dri | nking water | standards | | | | | | | 22 |

Chapter 1.

INTRODUCTION

Groundwater modelling is a technique to understand a system's response under certain conditions or to anticipate the system's future behaviour by representing it in another form. Groundwater modelling is an effective tool for groundwater resources management and protection. A logical relation between the info availability and model complexity should be considered for better presentation. When there's a shortage of data, selecting complex systems wouldn't end in desirable results and wouldn't show the real scenario. In such situations, we should review our expectations of the model's ability as per the data availability and accessibility. Representation of the real-world problem in simple form without compromising the accuracy is a challenge for the modellers. To get the best description of the real-world situations modellers tend to get the maximum data possible and the selection of the right model tool plays a vital role in the best representation of reality also. Classification of groundwater models can be done as a physical model, analogue model, and mathematical model. Physical models are the laboratory portrayal of the groundwater system such as the Sand tank which poses a scaling problem. Analogue models are the electronics models developed by the analogy between water flow systems and electrical flow systems (Delleur, 2006). For example, "Electrical current flow through a circuit board with resistors to represent hydraulic conductivity and capacitors as storage coefficient".

Representation of the groundwater system mathematically by a set of equations is known as a mathematical model. The mathematical models can be solved either numerically or analytically. Through the ages, analytical methods have become standard tools for explaining groundwater quantity and quality dynamics. Also, these models are occasionally applied before a numerical model starts. These models have their disadvantages concerning mathematical assumptions that may not occur naturally. Another problem is that they do not allow for simulating spatial and temporal variations in various parameters simultaneously. Hence, these models are often inadequate to mimic a heterogeneous subsurface system closely. "Numerical solutions can handle more complicated problems than analytical solutions. With the rapid development of computer processors and increasing speed, numerical modelling has become more effective and manageable"(Baalousha, 2005). A detailed explanation of numerical techniques is provided in the next sections.

1.1 Numerical Models

The finite difference method and the finite element method are the most commonly used approaches to solve the governing groundwater flow or solute transport equations numerically" (Wang et al., 2019). The modelling approach to be selected depends upon the modelling objectives and concerning problems. "The finite difference method can produce different results than the finite element method if the concern is complicated"(Baalousha, 2005). The modelling approach isn't the solitary factor that influences the outcomes of the model. Different elements such as initial conditions, boundary conditions, space discretization, and nature of information impact the outcomes. With numerical modelling, hydrogeologists could approximate the solutions of complicated differential equations of the system by converting them to discrete equations and dissecting the domain into meshes or grids. In numerical models, the dissection of a region and the discretization of differential equations are generally accomplished using approximation approaches like finite difference, finite element, and finite volume boundary. Each of these approaches can be applied solely or combined with other methods to reduce numerical models' computational complexity. Considering the applicability, ease of use, performance, and computational speed, each method has its limitations and advantages.

1.1.1 Finite Difference Method

"The finite difference method (FDM) has been widely used in groundwater studies since the early 1960s. FDM was studied by Newton, Gauss, Bessel, and Laplace" (Pinder and Gray, 1978).

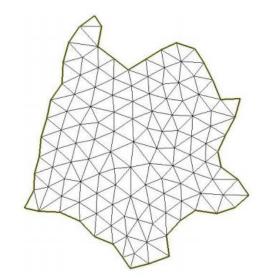
The finite-difference approximation is given by:

The finite difference method relies upon the calculation of a "function derivative by a finite-difference". In this method, the area of concern is divided into small cells of regular shape or grid points called nodes, the derivatives of the partial differential equations are approximated in space, concerning the differences between values of variables at adjacent cells or nodes. The nodes represent the specific values of the system's computational properties (e.g., hydraulic head, solute concentration, effective porosity) as functions of time. All nodes are defined in a body-fitted coordinate system and labelled consecutively by a set of indices (i, j, and k along the direction x, y, and z respectively). Discretization of the area in the finite difference method within a model domain is presented in figure 2.1. FDM is well documented easy to implement and gives reasonably good results. The main limitation of the finite difference method is that we cannot apply it appropriately to the irregular shape boundaries as the area of concern is divided into regular shape cells. Accuracy and the efforts required for computation are positively affected by the grid size and their distribution. "The output accuracy of the finite difference method is useful in

the case of solute transport modelling. Mass balance is not guaranteed if conductivity or grid spacing varies" (Baalousha, 2005).



Figure 1.1 Discretization of space in FDM





Source- (Elango, 2005)

1.1.2 Finite element method

FEM was initially used to solve problems related to civil engineering and construction. In this method, the grid is discretized into a network of nodes that form the vertices of irregularly/regularly-sized triangular elements. These elements and nodes are used to estimate the value of the field parameters like the solute concentration and hydraulic head. The elements may have different sizes, orientations and spatial dimensions. The mesh design is fundamental in the FEM because it greatly affects the solution's accuracy and convergence. The different approaches to the finite element method are Galerkin's method, weighted residuals, essential functions and variational principle (Pinder G., 1978). The key drawbacks of the method of finite elements over finite difference techniques are their complexity to formulate, difficulty to solve, and time to use. Conversely, to approximate a geometrically irregular mesh, these methods have more versatility than finite difference methods. However, to estimate an unconditionally irregular scheme, a large amount of calculation and storage memory for software simulation is required. "Advantages of this method include: a better mesh configuration, which suites irregular model boundaries, anisotropy is well incorporated, the governing system of equations is symmetric and irregular shapes can represent elements" (Baalousha, 2005). Discretization of the area in the finite element method within the domain of the model is shown in fig 2.2.

Chapter 2.

LITERATURE REVIEW

2.1 Migration of Solutes in Groundwater

From a variety of sources, contaminants are mobilised and released into the groundwater. Advection, advection-dispersion, and advection-dispersion-chemical/biological reaction models are typical solute transport models (Saatsaz, 2020). Advection models are defined as the solute's movement through groundwater flow, where there is no change in the solute concentration with distance. "Advection is primarily due to the effective porosity, hydraulic conductivity, and hydraulic gradient of the medium, according to Darcy's law of groundwater flow". When solute concentration changes in time and space due to diffusion and dispersion, advection-dispersion models are used to explain solute transport. The diffusion dispersion principle is used in these models. The word "dispersion" refers to a mechanical mixing process induced by the medium's heterogeneity. Solutes can spread in both longitudinal and transverse directions. The rate at which solute mixes by convergence and divergence of molecular diffusion and flow paths is determined by the saturation degree and the value of water velocity in porous media. When individual solutes shift slowly from a higher concentration region to a lower concentration region is called diffusion. Random molecular motions caused by the concentration gradient, with or without water movement, carry out this operation.

Models of advection-dispersion-chemical/biological reactions are by far more complicated. When chemical or biological reactions are introduced into advection-dispersion systems, these models are often used to measure the change in contaminants' concentration.

2.1.1 Governing Equations

The governing partial differential equations of contaminants transport can be expressed as follows (Zheng & Wang, 1998).

$$\frac{\partial}{\partial x} \left(w D_{xx} \frac{\partial c}{\partial x} + w D_{xy} \frac{\partial c}{\partial y} + w D_{xz} \frac{\partial c}{\partial z} \right) + \frac{\partial}{\partial y} \left(w D_{yy} \frac{\partial c}{\partial y} + w D_{yx} \frac{\partial c}{\partial x} + w D_{yz} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial z} \left(w D_{zz} \frac{\partial c}{\partial z} + w D_{zy} \frac{\partial c}{\partial y} + w D_{zx} \frac{\partial c}{\partial x} \right) - \left(q_x \frac{\partial c}{\partial x} + q_y \frac{\partial c}{\partial y} + q_z \frac{\partial c}{\partial z} \right) = \rho_b \frac{\partial s}{\partial t} + \frac{\partial w c}{\partial t} + K_m w C^m \pm R \dots Equation 2.1$$

Where w is the moisture content, D_{ij} (ij = x, y, z) is the hydrodynamic dispersion coefficient, c is the concentration of contaminants dissolved in water, q_x , q_y , q_z , are the groundwater velocities in x, y, z directions respectively and

$$q_x = -K_x \frac{\partial h}{\partial x}$$
, $q_y = -K_y \frac{\partial h}{\partial y}$, $q_z = -K_z \frac{\partial h}{\partial z}$

h is the hydraulic head, ρ_b is the bulk dry density of porous media, s is the weight of the adsorbed water per unit area of porous media, m is the order of chemical/biological decay, K_m is the contaminant concentration decay coefficient, R is the retardation coefficient and

$$R = 1 + \frac{\rho_b}{n} K_d.... Equation 2.2$$

Where n is the effective porosity and K_d is the partition coefficient. Hydrodynamic dispersion coefficient for isotropic porous media can be calculated by equations given below.

Where D_{xx} , D_{yy} , D_{zz} = Principal components of dispersion coefficient, D_{xy} , D_{xz} , D_{zx} , D_{zx} , $D_{zy}D_{yz}$ = Cross-terms of dispersion coefficient, ε_L = Longitudinal dispersivity, ε_T = Transeverse dispersivity, D^* = Effective molecular diffusion coefficient, v_x , v_z , v_y are velocity vector components along x,y and z axes, and v^2 = $v_x^2 + v_y^2 + v_z^2$; v is the magnitude of the velocity vector. The equation of the movement of groundwater through porous media is represented by Darcy's law as follow

$$\frac{\partial}{\partial x}(K_{xx}\frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - Q = S_s\frac{\partial h}{\partial t}\dots \dots Equation 2.9$$

Where, h = hydraulic head, $S_s =$ specific storage (volume of water released from the storage per unit volume of porous material per unit change in the head (flow area × Thickness), and K_{xx} , K_{yy} and K_{zz} are the hydraulic conductivities along the x, y and z axes. Q is the volumetric water flux (recharge/discharge) per unit volume of porous media (sources and sinks).

$$Q = \sum_{i=1}^{r} Q_i S(x - x_i)(y - y_i)(z - z_i)$$
 Equation 2.10

Where, S = number of sources and sinks along the x, y, z axes, Q_i is the volumetric injection/discharge rate at point (x_i, y_i, z_i) . The value of Q_i in withdrawal/discharging points is positive and for injection/recharging points is negative. More details about the above equations can be found in (Zheng & Wang, 1998) and (Harbaugh, 2005).

2.2 Modelling Approach

Identification of model objectives is the first step in any modelling. A critical concern in the modelling process is data collection and processing. However, model conceptualization is the most fundamental step in modelling. After completion of the model and the first run, calibration, verification, and sensitivity analysis can be performed. The steps involved in groundwater modelling are shown in Figure 2.1.

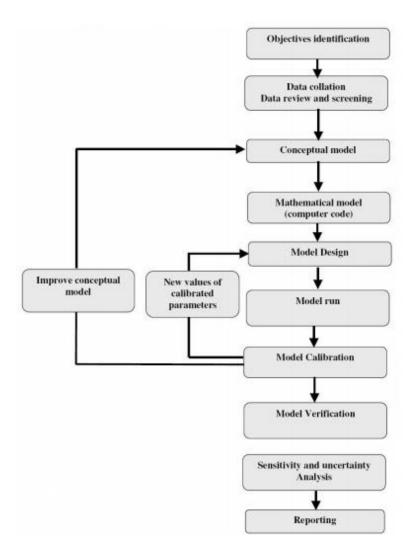


Figure 2.1 Modelling process flow chart(Baalousha, 2005)

2.2.1 Formulating modelling objectives

Objectives of modelling define the purpose of modelling. It guides the overall working of a model. Generally, management decisions on the quality or quantity of groundwater are based on the groundwater models. The model scope, methodology, and model type can differ depending on the modelling objectives. Groundwater models can be interpretive, predictive or generic. To study a specific case and to evaluate groundwater flow or the transport of pollutants, interpretive models are used. Predictive models, on the other hand, are used to know the difference in solute concentration or potential groundwater head. Different problems in the management of the water resources or remediation operations are studied using generic models.

Groundwater modelling objectives may be the measurement of groundwater flow and groundwater head, the investigation of the groundwater abstraction effect on the flow system at a well, the analysis of the effects on groundwater quality due to human activities (e.g. landfills, wastewater discharge, agricultural processes), or solute transport estimations. Modelling objective helps in model approach selection and collection of data needed.

2.2.2 Conceptual Model

Model conceptualization is a qualitative description of a ground-water system that includes the information of the water balance, hydrological and geological conditions. Model conceptualization is the most important part of groundwater modelling. After the identification of model objectives, it is the next step in the model development. Data about Geology, hydrology, boundary conditions and hydraulic parameters are needed to develop a conceptual model. A good conceptual model must be able to represent realworld situations in a simple manner that meets modelling goals and management requirements. In the case of groundwater quality modelling, it must outline our interpretation of contaminant transport or water flow.

The key factors that the conceptual model should contain are:

- Model domain area
- Aquifer's geometry
- Sources and sinks identification
- Groundwater recharge
- Boundary conditions
- Aquifer properties like Porosity, Hydraulic conductivity, Storativity
- Water balance

The mathematical model can be created after the completing model conceptualization. The mathematical model illustrates the assumptions made in the mathematical equations as well as the conceptual model. We can solve these equations either numerically or analytically.

2.2.3 Boundary Value Problem

The water balance theory underpins all mathematical models of groundwater flow. "In isotropic, homogeneous porous media, the general equation that governs three-dimensional groundwater steady-flow is

$$\frac{d^2h}{dx^2} + \frac{d^2h}{dy^2} + \frac{d^2h}{dz^2} = 0.\dots$$
 Equation 2.11

where h is the groundwater head". This equation is also known as the Laplace equation. The governing equation for groundwater flow is created by combining the "mass balance equation and Darcy's Law". To get a unique solution to an equation, we need to understand the boundary conditions. As a result, this equation is referred to as a "boundary value problem". So, the conditions at boundaries define the field or domain in which the "boundary value problem" can be solved.

2.2.3.1 Boundary Conditions

The first step in model conceptualization is to identify conditions at the boundaries. To get a peculiar solution to partial differential groundwater flow equations, boundary conditions must be identified. Improper boundary condition detection has an impact on the solution and can lead to completely incorrect output.

Three main types of boundary conditions are as follow:

- 1. Specified flow (also known as type II boundary or Neumann). Mathematically, $\nabla h(\mathcal{X}, \mathcal{Y}, \mathcal{Z}, \mathcal{T}) = \text{constant.}$
- 2. Specified head (also known as type I boundary or Dirichlet). Mathematically, it can be expressed as $h(\mathcal{X}, \mathcal{Y}, \mathcal{Z}, \mathcal{T}) = \text{constant.}$
- 3. Head dependent flow (also known as type III boundary or Cauchy). Mathematically it can be written as: $\nabla h(\mathcal{X}, \mathcal{Y}, \mathcal{Z}, \mathcal{T}) + a^*h = \text{constant}$ (where "a" is a constant). Natural boundaries should be identified carefully.

For example, Hydraulic boundaries, such as groundwater divides, may shift location as field conditions alter.

2.2.4 Selection of modelling software

The software for the modelling is selected after the hydrogeological characterization of the concerned area has been completed and the conceptual model has been created. The chosen model should have the potential to simulate the conditions at a given location. When field evidence shows that transport processes or groundwater flow are comparatively straightforward, analytical models can be used. Similarly, we can make use of model conceptualization and hydrogeological characterization to pick onedimensional, two-dimensional, or three-dimensional transport and groundwater flow models.

2.2.5 Model Design

Model designing includes all the input parameters that are needed to calibrate the model are included in the designing model. Degradation rate coefficients, dispersion coefficients transient or steady-state modelling, recharge, hydraulic conductivity/transmissivity, boundary conditions, layer elevations, model grid size and spacing, and any additional model data are all examples of input parameters.

2.2.6 Model Calibration

Calibration of the model is a method of fine-tuning the model results to fit the field measurements. Model results can vary from field measurements after the first run because modelling is merely a generalisation of the real world and estimations. So, errors in the computation are bound to occur. Model calibration is done by altering the model input parameter values to meet field conditions under certain limits. Field conditions at a site must be correctly defined before a model can be calibrated. A model calibrated to a set of conditions that do not represent real field conditions may result from a lack of proper site characterization. A model can be calibrated either automatically or manually. "PEST (Doherty et. Al. 1994) and UCODE (Poeter and Hill, 1994) are the software used for automatic calibration".

2.2.7 Model Verification

To meet historical field conditions, selected values of hydrogeological parameters, boundary conditions, sources, and sinks are used by a calibrated model. The model could be calibrated or refined further as a result of the verification process. Model verification is used to see if the calibrated model performs satisfactorily on any dataset or not. Since the calibration phase entails adjusting various parameters including recharge, pumping rate, hydraulic conductivity among other factors. As a result, different values for these parameters can yield a similar output. The model is ready for predictive simulations once it has successfully replicated measured changes in field conditions.

2.2.8 Sensitivity Analysis

There are a lot of uncertain parameters in regional groundwater models. It takes a long time and a lot of work to deal with these uncertainties. Sensitivity analysis identifies which parameters or a parameter has the greatest impact on the result. The process of changing values of input parameters of a model over a fair range (limits of uncertainty in the values of the model parameters) and examining the respective difference in model output is known as a sensitivity analysis. Observed changes in the contaminant transport, flow rate, or hydraulic head are usually recorded. Instead of parameters for which the model is comparatively insensitive, parameters for which the model is relatively responsive will necessitate future characterization.

2.2.9 Uncertainty Analysis

Any type of modelling is no better than an estimate due to uncertainties and errors in contaminant transport modelling groundwater flow modelling. For a variety of factors, uncertainty in groundwater modelling is unavoidable. Aquifer heterogeneity is one cause of uncertainty. Uncertainty exists in field data as well. "Mathematical modelling implies many assumptions and estimations, which increase the uncertainty of the model output" (Baalousha & Köngeter, 2006).

Any potential groundwater flow or contaminant transport conditions can be predicted using a model. The model can also be used to evaluate various problem mitigation options. As a result, all model predictions must be manifested as a set of potential outcomes, considering the uncertainties and assumptions made in model parameters and model input data.

2.3 Simulator Softwares for Transportation and Ground water flow modelling

2.3.1 MODFLOW Software (USGS Modular 3-Dimensional Groundwater Flow Mode)

The MODFLOW is the "most commonly used numerical groundwater flow model" (Kumar, 2012). The US Geological Survey created this three-dimensional model. It is used for saturated zones only and is based on the finite difference method. Numerous data preparation facilities, simple data exchange in standard form, extensive global experience, continuous growth, a relatively low price and source code availability are the advantages of MODFLOW(Kumar, 2003).

MODFLOW employs a block-centered finite-difference technique in the simulation of groundwater flow within the aquifer. The layers may be confined, unconfined or composition of both. Stresses due to external forces including evapotranspiration, areal recharge, flow to wells, flow to drains, and flow through riverbeds can all be modelled. However, unsaturated flow and surface runoff are not included in MODFLOW. So, MODFLOW cannot be used in the problems where the "flux at the groundwater table is dependent on the measured head and we do not know the function in advance" (Harbaugh, 2005).

Visual MODFLOW is one of the user-friendly and most important simulation environments to simulate three-dimensional contaminant transport and groundwater flow. The software's instructions were simple, and it could only simulate groundwater flow below the water table, according to the instructions. MODFLOWSURFACT, MODFLOW, ZoneBudget, MODPATH, MGO WinPEST and MT3D/RT3D, are all included in the Visual MODFLOW software kit with graphical user interface (Fouad et al., 2018). The MT3DMS is a three-dimensional numerical model that can be used to simulate solute transport in complicated hydrogeologic settings. It is MODFLOW's 3-D advection, dispersion, sorption, and reaction simulation module. It can be used in both saturated and unsaturated areas. MT3DMS can also simulate heat transfer in the presence of minor buoyancy and viscosity changes. In MT3DMS, chemical reactions such as advection-dispersion and diffusion are involved. It was created using the Finite Difference Method by (Chunmiao Zheng, 1990). Specifically designed to manage "advectively-dominated transport problems without the need to construct refined models for solute transport".

MODFLOW includes another module called RT3D, which is a three-dimensional solute reactive transport model (Clement, 1997). RT3D is used to solve linked partial differential equations describing the transport of multiple and immobile contaminants or species in saturated groundwater systems. Battelle Pacific Northwest National Laboratory developed RT3D (Reactive Transport Modelling in 3D with GMS) employs the FDM (Finite Difference Method). It's a tweaked version of MT3DMS that incorporates several reactive chemical packages. RT3D is capable of accurately simulating natural dilution and bioremediation.

2.3.2 FEFLOW (finite element subsurface and transport system)

The federal institute of geoscience (BGR) collaborated with the Institute of Hydromechanics (University of Hannover) to create a fractured rock simulation in the mid-1980s. To implement the flow process in complicated geological structures, RockFlow was created using a multi-dimensional finite element method. The Academy of Science (Chemnitz) created the FEFLOW code for "density-dependent flow processes in porous media" at the same time. At the time, FORTRAN code was used to implement RockFlow and FEFLOW. Groundwater flows and contaminant transport can be simulated in 2D and 3D using a finite element subsurface and transport system (FEFLOW)(Koukidou & Panagopoulos, 2010). Also, it can simulate flow for groundwater age, heat and mass transport in both transient and steady-state modes. FEFLOW is well-suited to salinity and heat-dependent transport. It is a powerful tool for describing the spatial and temporal distribution and reactions of contaminants in groundwater(*FEFLOW* 7.3).

It is capable of computing:

- 1. The processes related to geothermal energy
- 2. The total period and travel duration of the contaminant in aquifers
- 3. Ground-water systems with and without free surfaces like perched aquifers, phreatic aquifers, moving meshes
- 4. Thermohaline flows (Both temperature and salinity dependent transport phenomena)
- 5. Saturated-unsaturated zone problems

6. Complex parametric and geometric situations.

This program is completely interactive and graphics-based. The pre-, main-, and postprocessing stages are all combined. A data interface and a programming interface are available for GIS (Geographic Information System).

The workflow of FEFLOW and MODFLOW based on the conceptual model is shown in figure 2.2.

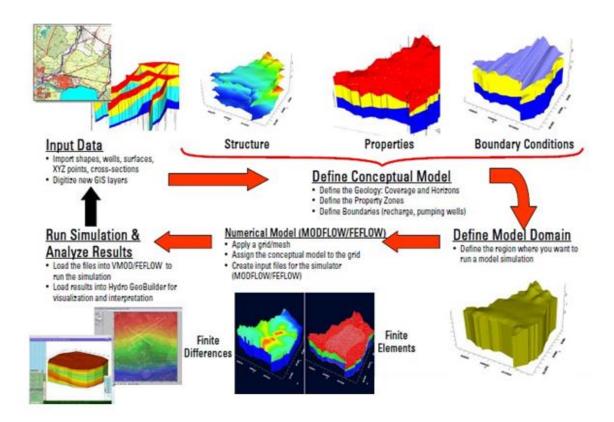


Figure 2.2 Workflow of FEFLOW and MODFLOW (Fouad et al., 2018)

2.3.3 HST3D (3-D Heat and Solute Transport Model)

HST3D (Heat and Solute Transport Model) is used to simulate groundwater flow and related heat and solute transport in 3D form. It is an effective and user-friendly interface built into the Argus ONE (Argus Open Numerical Environments) modelling environment. Users can input all spatial data, run HST3D graphically, and visualize the output using HST3D. Within one comprehensive graphical user interface (GUI) Argus ONE incorporates GIS, CAD, Database, Geostatistics, Conceptual Modelling, Automated Grid and Mesh Creation, and Scientific Visualization(Kipp, 1997). The HST3D model can be used to examine issues such as – freshwater recharge and recovery, contaminant plume movement, subsurface waste injection, landfill leaching, geothermal water systems, hazardous waste disposal, the intrusion of saltwater, subsurface energy

storage and other transportation-related issues (Kumar, 2012). To run HST3D, you'll need the Argus ONE GIS and Grid Modules. Only the heat- or solute-transport equation is solved in combination with the ground-water flow in most applications.

2.3.4 SUTRA (3-D Saturated/Unsaturated Transport Model)

"SUTRA is a finite-element simulation model for saturated - unsaturated, fluid-densitydependent ground-water flow with energy transport or chemically-reactive single-species solute transport with energy transport" (Souza et.*al*, 1987). For saturated groundwater flow zones, SUTRA may be used for cross-sectional and areal modelling and crosssectional modelling of unsaturated flow systems. "Solute transport simulation with SUTRA can be used to model natural or man-made chemical species transport, including solute sorption, production and decay processes, as well as to analyse ground-water pollutant transport problems and aquifer reclamation designs". SUTRA can model "variable density leachate movement" and "cross-sectional modelling of saltwater intrusion in aquifers" at regional scales and near-well, with either dispersed or rather sharp transition zones between saltwater and freshwater.

To solve the governing equations describing the two interdependent processes that are simulated, the model uses a "three-dimensional hybrid finite element and integrated finite difference technique". The approximation is done for the governing equations of unsaturated or saturated ground-water flow dependent on fluid density, and either

(a) transport of a contaminant in the groundwater, where contaminant can be subjected to equilibrium adsorption on the porous matrix with both first-order and zero-order production or decay, or

(b) transport of thermal energy in the groundwater and solid matrix of the aquifer.

2.3.5 Use of GIS and Meshfree techniques

With the aid of various geo analysts and spatial statistical methods, a large number of GIS-based systems have been used in recent years to classify regions vulnerable to contamination (Shrimali et.al, 2019). QGIS, ArcGIS Model Builder and Visual Basics (VB) software can be used to develop a GIS-based Contaminant Transport Model (GIS-CONTRAM) to demonstrate the fate of contaminants transport in the subsurface (Menezes, 2009). Also, GIS tools can be used to create iso-concentration contour maps showing spatial distribution of contaminants. These maps will assist in groundwater quality assessment and help in visualisation of sites having high or low contaminants concentrations. A case study of spatial analysis of groundwater quality is done using the QGIS software in this research. QGIS is an open source software.

When checked with Visual MODFLOW, the CONTRAM model achieved fair results. The element free Galerkin method (EFGM) is a sufficiently accurate and simple method for numerically simulating contaminant transport in two dimensions through saturated homogeneous porous media and landfill liners. In the EFGM, an estimated solution is designed entirely in terms of a series of nodes, and no characterization of the nodes interrelationship is needed. The EFGM approximates the function with moving

least square approximants and imposes critical boundary conditions with the Lagrange multiplier process. The EFGM findings and the data from the field investigation are in good agreement(Praveen Kumar & Dodagoudar, 2009).

Chapter 3.

METHODOLOGY

With the rapid development of the population, urbanisation, and agriculture, industrialization has brought about water pollution, which is one of the greatest threats facing the environment today. In Uttar Pradesh, the need for water is always increasing. More than one billion people around the world still lack access to an enough and secure water supply, with more than 800 million of them living in rural areas. Groundwater is used as raw water for 85 per cent of India's public water supply (WHO, 1998). Only 38% of the nearly 2.5 billion people in developing countries had safe drinking water in the 1970s. Water supply coverage was 75 per cent in urban areas and 46 per cent in rural regions at the start of the 1980s.

Groundwater quality can deteriorate for a variety of causes. The first is excessive withdrawals without long-term planning. Other factors include the haphazard construction of cities. Other factors include sewage spillage due to broken or outdated infrastructure, random transfer of home and industrial waste into the ground, saltwater intrusion, and incorrect use of agricultural pesticides (Hem, 1985). Because of the increased demand for food grains, more fertilisers and pesticides are utilised, which soak into the soil and pollute ground water. Because many companies dump their effluent onto open lands due to high costs of dilution and insufficient sewage treatment facilities, effective and profitable exploitation of the industries' effluents requires further attention.

The drying of surface water and the decrease of groundwater levels have exacerbated a water crisis in the Mathura region of Uttar Pradesh, India. Salt intrusion, soil salinization, and, most critically, contamination result from excessive groundwater abstraction for irrigation and poor fertiliser practices. Using the IDW interpolation tool in QGIS, this study seeks to find prospective groundwater prospect zones that are safe for drinking and irrigation in the Mathura district. According to the Central Ground Water Board of India, this region has 61456 tube wells and borewells. Pre-monsoon water levels range from 2.65 to 14.34 m below ground level (bgl), whereas post-monsoon levels range from 1.33 to 14.0 m bgl (Sant Lal, 2012).

The groundwater data for 20 locations from different parts of the Mathura district is taken from the CGWB website. The data contains 11 Physico-chemical properties of water namely Calcium(mg/l), Chlorides(mg/l), Electrical conductivity(µmhos/cm), Fluorides(mg/l), Bicarbonates(mg/l), Magnesium(mg/l), Nitrates(mg/l), pH values, Sulphates(mg/l), Total dissolved solids(mg/l), Total hardness(mg/l). Locations for which data is taken are Baldeo, Barsana, Chaumuhan, Chhata, Farah, Goverdhan, Jachoda, Jhinga Nagla, Kosi, Mat, Naujheel, Paintha Goverdhan, Palson Gaon, Raya, Sahar1, Saunkh, Surir (new) and Vrindavan. Assessment of the physio-chemical parameters for groundwater is done by comparing it with standard values recommended by the WHO and BIS.

The spatial distribution maps of the Physico-chemical properties of water were created using the QGIS application. In QGIS, the iso-concentration contour maps are created using the Inverse distance weighting (IDW) interpolation method. The interpolation technique was adopted using the extension within the QGIS environment.

The Inverse Distance Weighting interpolator assumes that each input point has a local influence that diminishes with distance. It weights the points closer to the processing cell greater than those further away. A specified number of points, or all points within a specified radius can be used to determine the output value of each location. Use of this method assumes the variable being mapped decreases in influence with distance from its sampled location. The Inverse Distance Weighting (IDW) algorithm effectively is a moving average interpolator that is usually applied to highly variable data. For certain data types it is possible to return to the collection site and record a new value that is statistically different from the original reading but within the general trend for the area.

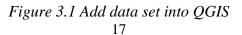
IDW interpolation explicitly implements the assumption that things that are close to one another are more alike than those that are farther apart. To predict a value for any unmeasured location, IDW will use the measured values surrounding the prediction location. Those measured values closest to the prediction location will have more influence on the predicted value than those farther away. Thus, IDW assumes that each measured point has a local influence that diminishes with distance. The IDW function should be used when the set of points is dense enough to capture the extent of local surface variation needed for analysis. IDW determines cell values using a linear-weighted combination set of sample points. It weights the points closer to the prediction location greater than those farther away, hence the name inverse distance weighted.

The IDW technique calculates a value for each grid node by examining surrounding data points that lie within a user-defined search radius. Some or all the data points can be used in the interpolation process. The node value is calculated by averaging the weighted sum of all the points. Data points that lie progressively farther from the node influence the computed value far less than those lying closer to the node.

3.1 Steps involved in interpolation

After downloading the raw data from CGWB website, cleaning of data was done using Microsoft excel. Latitude and longitudes were added manually and file format to save the data was selected as .csv. After the dataset is ready, it is added to QGIS map canvas. Select Data source Manager, then select Delimited Dataset. On the Filename, browse and select the data. Next specify the field for Point coordinates which is column X co-ordinate and Y co-ordinate for X and Y. The coordinates are in meter in local system (there is no information about the coordinate system used in the dataset, so local coordinate system is assumed in this research). Because there is no information about coordinate system for the dataset, so this research uses World Mercator Coordinate System (EPSG: 4326). Below the Sample data preview, you can see how the data looks like. If you see the data is separated well for each column, then everything is fine. Lastly select Add button to add the data into QGIS and close the Data source Manager window.

| Q | Data Source Mar | iager Delimi | ted Text | | | | | | | | | | | | | | | | | |
|--------------|-------------------|----------------|---------------------------------|--------------------|------------|-------------|-------------|------|----|---------|---------|---------------|-----------|--------------|------------|--------------|---------------|-------------|---|---------|
| | Browser | File name | C: \Users \man | nu\Desktop | o\Groundwa | ter qua | lity data | .CSV | | | | | | | | | | | ¢ | |
| V | Vector | Layer name | Groundwat | er quality d | ata | | | | | | | | | Enc | oding (| ЛТF-8 | | | | - |
| ٥, | Raster | ▼ File | Format | | | | | | | | | | | | | | | | | |
| | | | SV (comma se | | | | | | | | | | | | | | | | | |
| 9 | Delimited Text | | egular expres ustom delimite | | er | | | | | | | | | | | | | | | |
| | GeoPackage | Receiption | ord and Fiel | lds Option | s | | | | | | | | | | | | | | | |
| P. | SpatiaLite | 🖝 Geo | metry Defi | nition | | | | | | | | | | | | | | | | |
| Ф. | PostgreSQL | • Po | oint coordinat | es | | X field | Longitu | ıde | | | | | | ▼ Z | field | | | | | - |
|)))) | MSSQL | 0 w | ell known tex | t (WKT) | | Y field | Latitud | | | | | | | ▼ M | field | | | | | • |
| | Oracle | | o geometry (a | attribute on | ly table) | Geome | try CRS | EPSG | | - WGS 8 | 34 | | | | | | | | • | ۵ |
| DB2 | DB2 | ▶ Laye | er Settings | | | | | | | | | | | | | | | | | |
| V | Virtual Layer | Sample | Data | | | | | | | | | | | | | | | | | |
| () | WMS/WMTS | | | | Longitude | | TH | f | ec | tds | NO3 | CI | Ca | Mg | _ | SO4 | HCO3 | | | |
| | WES LOCC | | | 27.4194 27.6556 | | 8.43 8.1 | 176 1215 | | | | 9 27 | 21.27 1177 | 38 120 | 42.24 220 | 100 328 | 35.86 144 | 235.46 146 | | | _ |
| | API - | | haumuhan | | | 8.35 | 225 | | | | 13 | 284 | 16 | 45 | 319 | 170 | 329 | | | |
| | Features | | | 27.7333 | | 8.39 | 644 | | | | 9 | 248.15 | | 154.56 | _ | | 268.4 | | | * |
| | wcs | | | | | | | | | | | | | | | | | | | |
| | XYZ | • | | | | | | | | | | | | | | | Close | <u>A</u> dd | н | elp |



After the data is loaded into QGIS. Export the data into shape file format. It can be done by right click the point layer then select Export >> Save Feature As. The Save Vector Layer as... window will appear. Select the ESRI Shapefile for Format. In the File name specify a name and place where the exported data will be saved. For CRS use the same as previous one, World Mercator.

| 🔇 Save Vecto | or Layer a | 15 | | | | | > | < |
|---|------------|-------------|-------------------|--------|-------|--------|--------|---|
| | | | | | | | | |
| Format | GeoPac | age | | | | | • | |
| File name | shapefile | | | | | | | |
| Layer name | shapefile | • | | | | | | |
| CRS | EPSG:43 | 26 - WGS 84 | 4 | | | | • | |
| | | d features | | UTF-8 | | | Ţ | |
| Select Geome | | export an | d their export op | tions | | | | |
| Geometry | type | | | Auton | natic | | • | |
| Force | multi-typ | 2 | | | | | | |
| Includ | le z-dimen | sion | | | | | | |
| ▶ Ext | ent (cur | rent: none | .) | | | | | |
| ▼ Layer (| | | | | | | | |
| DESCRIPT | ION | | | | | | | |
| FID | | fid | | | | | | |
| GEOMETR | | geom | | | | | | |
| | | geom | | | | | | |
| IDENTIFIE | | | | | | | | |
| SPATIAL_I | INDEX | YES | | | | | • | |
| Custon | n Option | 5 | | | | | | |
| | | | ✓ Add saved file | to map | OK | Cancel | l Help |) |

Figure 3.2 Export data to shapefile

Now, we are ready to do the IDW interpolation. In QGIS we can do the IDW interpolation using three tools, there are: IDW Interpolation from QGIS Interpolation tool. v.surf.idw from GRASS and GRID (IDW Nearest Neighbour Searching) from

GDAL. If you type a keyword IDW, those three tools will appear in the processing toolbox as in figure.

| IDW Interpolation | | | | | | > |
|---------------------------------|------------------|----------------|------------------|------|------|------------|
| Parameters Log | | | | | | |
| Input layer(s) | | | | | | A |
| Vector layer | ° Groundw | ater quality o | lata | | | • |
| Interpolation attribute | 1.2 HCO3 | | | | | • |
| Use Z-coordinate f | or interpolation | | | | | |
| | | | | | | (+) |
| Vector layer A | Attribute | Туре | | | | |
| Groundwat H | HCO3 | Points | | | | - |
| | | | | | | |
| Distance coefficient P | | | | | | |
| 2.000000 | | | | | | \$ |
| Extent | | | | | | |
| 77.275779724,77.9715 | 19470,27.2390 | 59448,27.97 | 70514297 [EPSG:4 | 326] | | |
| Output raster size | | | | | | |
| | | Columns | 8 | \$ | | |
| Rows 8 | \$ | Columns | | | | |
| Rows 8 Pixel size X 0.100000 | | Pixel size Y | 0.100000 | \$ | | |
| | | | 0.100000 | | | |
| | | | 0.100000 | | | Cancel |

Figure 3.3 IDW interpolation

This research uses IDW interpolation tool from QGIS. From the processing toolbox, vector layer of groundwater quality data is added and interpolation attribute is selected, which is HCO_3 here in figure. Now click on plus button to add your vector layer with attributes. Then you can set some parameters like Weighting Power (*P* value). Higher value will give smoother result. Next, specify the extent, which is the field value to be interpolated. This project is to make the map for Mathura district, so chose the corresponding field. Then at bottom of the window tool, you can specify a place where the output will be saved. If you want to view the result before you save it, leave it as temporary file. Finally click Run button to start the interpolation. When done the result will be added to your QGIS map canvas.

The result in QGIS will be in grayscale mode. To make it more beautiful just customize the symbology. To do it, right click the output result and select Properties (Or simply

you can double click the layer name). The Layer Properties window will appear as in figure. Select Symbology. In the Band Rendering option change the Render type to Single band pseudo colour. Right away the output value will be classified into some classes with different colour. Of course, you can change the number of classes or change the colour, just explore if you want to.

| 📿 Laj | yer Properties — Inte | rpolated — Sy | mbology | | | | | | | | × | |
|------------|-----------------------|---------------|-----------|---------------|--------|-----|-----|--------|-----------------|--------|---|-----|
| Q | | | dering | | | | | | | | - | |
| <i>i</i> • | nformation | Render type | Singleban | d pseudocolor | • | | | | | | | T • |
| ာ့ န | Source | Band | | Band | 1 | | | | | - | | |
| | | Min | | 7.623 | 3933 | | Max | | 748.23853999999 | 999436 | | |
| « | Symbology | ▶ Min / M | 1ax Value | Settings | | | | | | | | |
| Т | Transparency | Interpolatio | n | | Linear | | | | | Ŧ | | |
| Ь | Histogram | Color ramp | | | | | | | | • | | [|
| R R | Rendering | Label unit s | uffix | | | | | | | | | |
| | - | Label precis | ion | | 4 | | | | | | | |
| 🕓 Т | Temporal | Value | C | olor Labe | 1 | | | | | | | |
| / 1 | Pyramids | 7.6233 | 3933 | 7.62 | 34 | | | | | | | |
| | Metadata | 139.87 | 760980 | 139. | 8761 | | | | | | | |
| | Legend QGIS Server | 735.01 | 132695 | 735. | 0133 | | | | | | | |
| | 2013 Server | | | | | | | | | | | |
| | | | | | | | | | | | - | |
| | | Style * | • | | | (| ОК | Cancel | Apply | Help | | |
| | | | | | | | | | | | | |
| | | | | | | - 6 | _ | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | i | | UK | | | nep | | |

Figure 3.4 Change symbology

3.2 Study Area

Mathura, one of Uttar Pradesh's most populous districts (2.5 million people), is an important site for Hindus (Census, 2011). The examined region is approximately 3339 square kilometres and is located between latitudes 27° 14′ and 27° 17′ N and longitudes 77° 17′ and 78° 12′ E. The average monthly maximum temperature ranges between 36°C and 47°C in the summer and 25°C and 32°C in the winter, with an annual rainfall of 826 mm (CGWB, 2012).

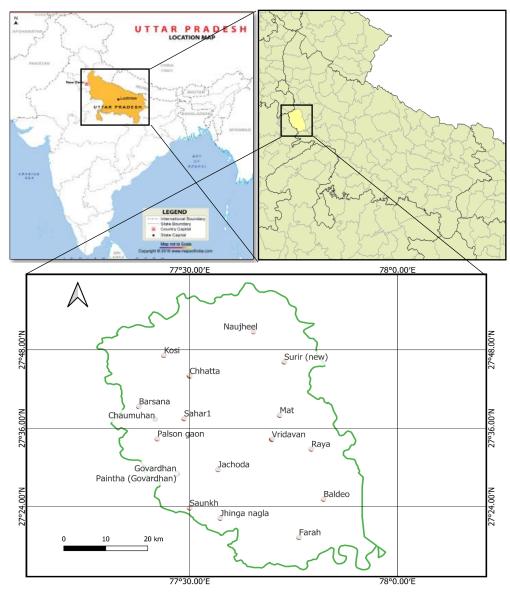


Figure 3.5 Location of study area and sites of groundwater samples in Mathura district India

The research area is covered by toposheets 54E and 54I as per the Survey of India. The Yamuna River, which joins the area from the north and flows in a meandering pattern and then enters the Agra district, is the only source of drainage in the area.

3.3 Analysis of data

Whisker plot and descriptive statistics of data set is shown in figure 3.6 and table 3.1 respectively. Whisker plot is a way of summarizing a set of data measured on an interval scale. It is often used in explanatory data analysis. In whisker plot the ends of the box are the upper and lower quartiles, so the box spans the interquartile range. the median is marked by a vertical line inside the box.

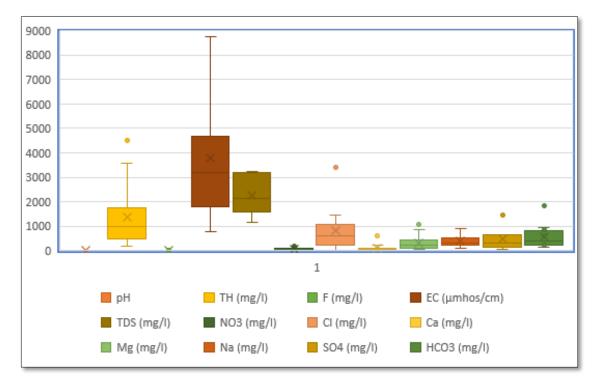


Figure 3.6 Whisker plot

Table 3.1 Descriptive statistics and range of parameters in groundwater samples andtheir comparison with drinking water standards

| | | | | mean | Standar | Standard | Minim | Maxim | Media | Confide |
|------------|----------|---------|-----------|------------|---------|----------|--------|---------|------------|---------|
| Parameters | WHO | BIS | 2012 | | d | Error | um | um | n | nce |
| | 2006 | | | | Deviati | | | | | Level |
| | | | | | on | | | | | (95.0%) |
| | Highest | Desira | Max | | | | | | | |
| | desirabl | ble | permissi | | | | | | | |
| | e limits | limit | ble limit | | | | | | | |
| | (mg/l) | (mg/l) | (mg/l) | | | | | | | |
| pН | 6.5-8.5 | 6.5-8.5 | | 8.13 | 0.23 | 0.06 | 7.66 | 8.43 | 8.10 | 0.14 |
| TH | 500 | 300 | 600 | 1387. | 1355.7 | 391.38 | 176.00 | 4526.00 | 999.0 | 861.42 |
| | 200 | 200 | 000 | 08 | 8 | 071100 | 170100 | .020100 | 0 | 0011.2 |
| F | 1 | 1 | 1.5 | 1.33 | 1.42 | 0.33 | 0.07 | 6.53 | 1.00 | 0.68 |
| EC(µmhos/ | 750 | | | 3798. | 2979.5 | 683.55 | 780.00 | 12920.0 | 3180. | 1436.08 |
| cm) | | | | 84 | 1 | | | 0 | 00 | |
| TDS | 500 | 500 | 2000 | 2257. | 834.30 | 340.60 | 1169.0 | 3229.00 | 2116. | 875.54 |
| | | | | 17 | | | 0 | | 50 | |
| NO3 | 45 | 45 | 100 | 55.02 | 80.02 | 23.10 | 2.20 | 239.00 | 17.00 | 50.84 |
| Cl | 250 | 250 | 1000 | 808.9 | 890.76 | 247.05 | 21.27 | 3403.20 | 616.8 | 538.28 |
| | | | | 1 | | | | | 3 | |
| Ca | 75 | 75 | 200 | 115.6 | 163.57 | 47.22 | 16.00 | 604.00 | 51.60 | 103.93 |
| | 20 | 20 | 100 | 7 | 220 51 | 05.41 | 12.24 | 1006.04 | 011.7 | 200.00 |
| Mg | 30 | 30 | 100 | 321.1 | 330.51 | 95.41 | 42.24 | 1086.24 | 211.7 | 209.99 |
| | 200 | | 200 | 7 | 225.05 | 60.11 | 100.00 | 000.00 | 6 | 140.01 |
| Na | 200 | | 200 | 387.4 | 235.95 | 68.11 | 100.00 | 900.00 | 323.5 | 149.91 |
| SO4 | 200 | 200 | 400 | 2 498.9 | 500.31 | 144.43 | 35.86 | 1490.00 | 0 297.0 | 317.88 |
| 304 | 200 | 200 | 400 | 498.9 9 | 500.51 | 144.43 | 55.80 | 1490.00 | 297.0 | 517.88 |
| НСО3 | 200 | 200 | 600 | - | 472.16 | 136.30 | 146.00 | 1832.44 | 390.8 | 300.00 |
| псоз | 200 | 200 | 000 | 576.8 3 | 472.10 | 150.50 | 140.00 | 1032.44 | 390.8 | 500.00 |
| | | | | 3 | | | | | 1 | |

Chapter 4.

RESULTS AND DISCUSSION

Previous research has suggested that the Indo-Gangetic plain's sodic soils are formed by in-situ weathering of alkali aluminosilicates (Kapoor et al. 1981). Salt-rich geological formations are also thought to have contributed to the Ganga plain's alluvial deposits (Kumar et al.1993). Magnesium and TDS are natural aquifer elements, thus the probability of them originating from the anthropogenic activity are slim. Figure 4.7 could explain the increased nitrate amounts. Agricultural land covers a substantial portion of the Mathura district. Improper nitrogen fertiliser application in agriculture areas could lead to nitrate contamination of the groundwater in Mathura and the surrounding regions. Other nitrogen sources, such as sewage effluents, natural soil, animal excreta, and their dilution owing to rainfall infiltration, should be considered as sources for the Mathura region.

4.1 Electrical conductivity

One of the most important physio-chemical characteristics influencing water quality is electrical conductivity, which is a measurement of water's ability to carry electrical current. The mean EC value in water samples is 3798.85 µmhos/cm, with a range of 780 to 12920 µmhos/cm. The ability of water to transmit electric current is defined as EC, with higher EC indicating salt content in the groundwater(Krishna kumar et al., 2015). EC in water can be classified into four types according to Indian classification: C1 (EC 250 (µmhos/cm); C2 (EC: 250 to 750 mhos/cm); C3 (EC 750 to 2250 mhos/cm); and C4 (EC > 2250 mhos/cm)(Vyas & Jethoo, 2015). Based on this classification of EC, none of the analysed groundwater samples falling under type II (C2), and 75% of the samples falling under the type III (C2) and 75% of the samples falling under type IV (C4). EC concentration ranges between 780 to 12920 µmhos/cm.

Figure 4.1 shows the iso-concentration contour lines for Electrical Conductivity (EC) analysed using inverse distance weight (IDW) interpolation in a GIS environment. The map is created using four colour bands. EC less than 250 mhos/cm, EC between 250-750 mhos/cm, EC between 750-2250 mhos/cm, and EC above 2250 mhos/cm are represented

by purple, light blue, blue, and green colours, respectively. The figure suggests that the EC concentration is beyond the allowed value for the entire district. Three blocks Sahar, Surir and Baldeo falls in the C3 category and the rest of the district falls in the C4 category. The CE map suggests that the water in the Mathura district is not suitable for irrigation uses.

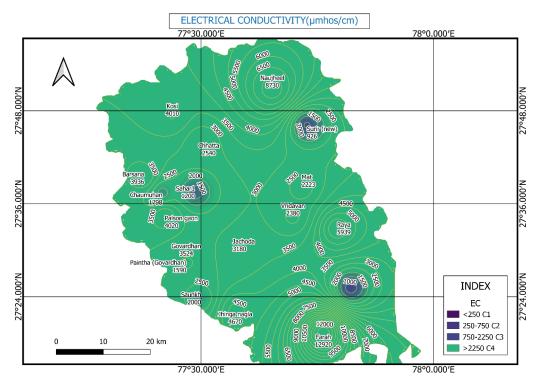


Figure 4.1 Iso-concentration map showing the spatial distribution of Electrical Conductivity

4.2 Total dissolved solids

Another key physio-chemical measure determining water quality is total dissolved solids (TDS). TDS may be defined as total inorganic salt concentration and a little quantity of organic salts dissolved in the water. The total dissolved solids (TDS) in groundwater samples ranged from 1169 mg/l to 3229 mg/l. TDS in drinking water, on the other hand, should be kept to a maximum of 500 mg/l(BIS, 2012). All the samples taken in this research area are above the allowed limit, suggesting serious contamination and a health risk.

Figure 4.2 shows the spatial distribution map of the TDS concentration. TDS concentration less than 500 mg/l is shown in purple, TDS between 500 and 200 mg/l is shown in green, and the yellow colour represents TDS greater than 2000 mg/l. It can be

seen in the figure that each block of Mathura district has TDS greater than desirable limits and the north-western part has TDS in between the desirable and maximum permissible range.

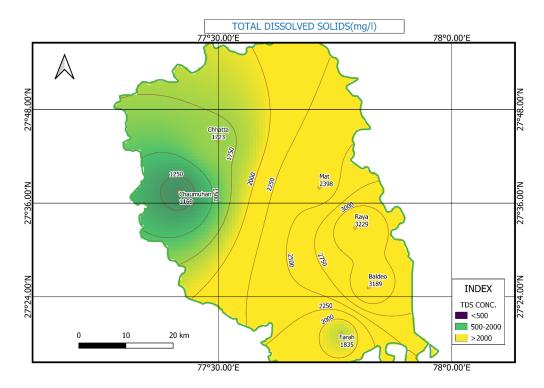


Figure 4.2 Iso-concentration map showing the spatial distribution of Total Dissolved Solids

4.3 Sodium

According to WHO regulations, sodium is the most prevalent component in common water, has an allowed level of 200 mg/l (WHO, 2008). Na+ concentrations in the collected samples range from 100 to 900 mg/l, with a mean of 387 mg/l. More than 75% of samples are found to be above the allowed limit. Salt deposition from silicate containing minerals and fertilisers may be to blame for the high amounts.

Figure 4.3 shows the contour lines of iso-concentration for sodium analysed using inverse distance weight (IDW) interpolation in a GIS environment. Sodium less than 200 mg/l is shown in brown and Na>200mg/l is shown in yellow. Sodium levels are more than the allowed limit in the entire area except for some patches in the south-eastern parts.

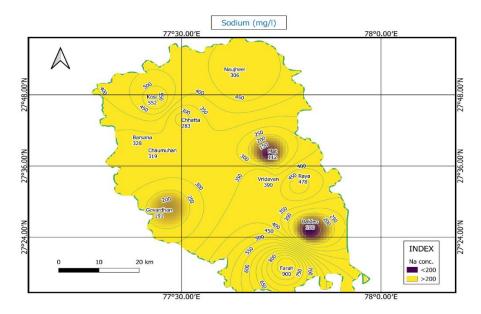


Figure 4.3 Iso-concentration map showing the spatial distribution of Sodium

4.4 Calcium

Calcium concentrations range from 16 mg/l to 604 mg/l, with a mean of 115.67 mg/l. Only about 17% of samples exceed the WHO's acceptable level of 200 mg/l.

The spatial distribution map of calcium is shown in Figure 4.4. Purple represents Calcium is within desirable limits, i.e. Ca < 75 mg/l, Calcium greater than the allowed limit of 200mg/l is shown in yellow, and the green represents the calcium concentration of 75-200 mg/l. It can be seen in figure 4.4, the area near the Baldeo site is yellow suggesting that calcium levels in that region are above the maximum allowed value but in central and north-western parts, the Calcium concentration is within desirable limits.

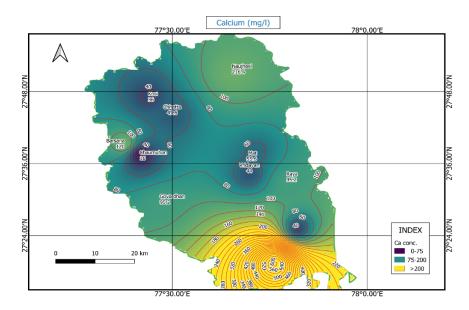


Figure 4.4 Iso-concentration map showing the Spatial distribution of Calcium

4.5 Magnesium

Magnesium levels in groundwater samples are extremely high. According to the data collected, most of the study region has a value in the non-permissible category (>30 mg/l). With a mean of 321 mg/l, it ranges from 42.24 mg/l to 1086.24 mg/l.

The spatial distribution map of Magnesium is shown in figure 4.5. Yellow colour represents an area having Mg concentration greater than 100 mg/l. The purple colour shows an area having Mg less than 30 mg/l and Mg between 30 and 100 is shown in green. It is clear from the map that Mg is above the limit of 30mg/l in the whole of Mathura except Baldeo and Chaumuhan where Mg concentration is between desirable and Maximum limit.

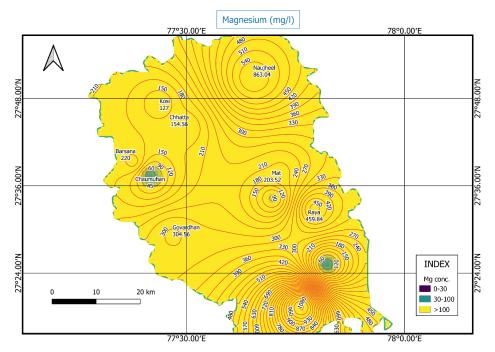


Figure 4.5 Iso-concentration map showing the spatial distribution of Magnesium

4.6 Total Hardness

The Total Hardness (TH) in the study area varies between 176 to 4526 mg/l with a mean value of 1387 mg/l. The WHO standard for TH is 500 mg/l. It suggests that 75% of collected water samples are unsuitable for drinking purposes. Iso-concentration map of Total Hardness is shown in figure 4.6. TH less than 200 mg/l is shown in purple, TH between 200-600 mg/l is shown in blue and yellow represents TH above 600 mg/l. Figure 4.6 suggests that total hardness is above the desirable limit in most parts of the Mathura except in some areas nearby the Baldeo, Raya and Chaumuhan.

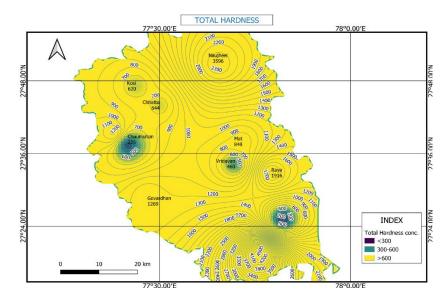


Figure 4.6 Iso-concentration map showing the spatial distribution of Total Hardness

4.7 Nitrate

The breakdown of organic materials, sewage waste, and fertiliser application all contribute to nitrate in groundwater. The concentration ranges from 2.2 to 239 mg/l in the study region. The spatial distribution map of nitrate is shown in Figure 4.7. Here, the purple colour represents the area having Nitrate concentration below 45 mg/l, yellow colour shows Nitrate greater than 100 mg/l, and nitrate concentration between 45-100 mg/l is shown in green colour. From figure 4.7, Nitrate concentration is alarming in the central blocks nearby Vrindavan and the northern part near the Naujheel1 site suggesting groundwater pollution in that area.

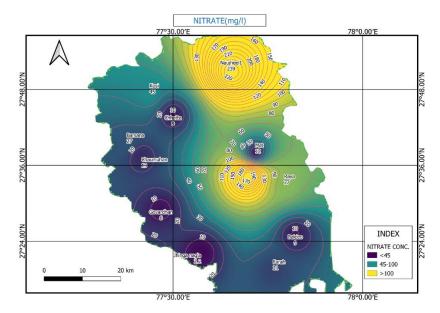


Figure 4.7 Iso-concentration map showing the spatial distribution of Nitrate

4.8 Sulphate

Sulphate is mostly made up of sulphide minerals that are found in igneous and metamorphic rocks. The sulphate ion is also produced by anhydrite in sedimentary rocks. Sulphate levels range from 35.86 mg/l to 1490 mg/l in the study region, with a mean of 499 mg/l. The allowable limit of 200 mg/l is exceeded in 75% of the samples. Figure 4.8 shows the iso-concentration contour lines for Sulphates analysed using inverse distance weight (IDW) interpolation in a GIS environment. Purple colour in spatial distribution map of Sulphates demonstrate area where Sulphate is less than 200 mg/l, sulphate concentration greater than 400 mg/l is shown in yellow, and green colour shows the area where sulphate concentration lies between 200-400 mg/l. It can be observed that the northern and southern parts of the study area have SO₄ levels above the prescribed limit.

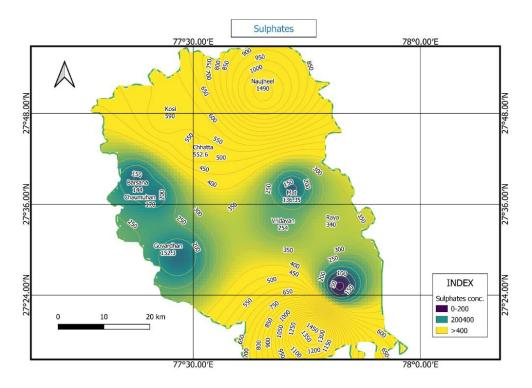


Figure 4.8 Iso-concentration map showing the spatial distribution of Sulphate

4.9 Bicarbonate

The chemical breakdown of carbonate rocks and some dissolved CO_2 in rainwater cause bicarbonate ion concentrations in water. HCO_3 concentrations range from 146 to 1832 mg/l, with a mean value of 576.83 mg/l exceeding the maximum allowed limit of 200 mg/l. In Figure 4.9. The spatial distribution of the bicarbonate data is shown, where purple is used for the area having bicarbonate levels below 200mg/l, Bicarbonate greater than 600 mg/l is shown in yellow and green to demonstrate the area having bicarbonate concentration between 200-600 mg/l. Figure 4.9 clearly shows that except Barsana on the western side, the entire district has Bicarbonate levels above the desired value.

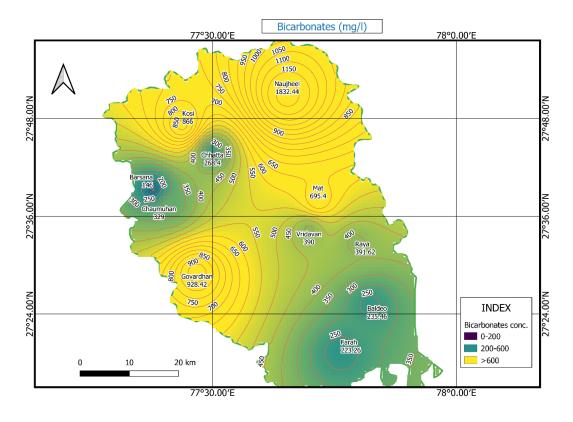


Figure 4.9 Iso-concentration map showing the spatial distribution of Bicarbonates

4.10 Chloride

Chloride salts are very soluble and do not react chemically with reservoir rock minerals, remaining in the form of sodium chloride. A high chloride content indicates a higher level of organic pollution. WHO (2008) established a maximum acceptable value of 250 mg/l.? The concentration of Cl in the study area varies between 21.27 mg/l and 3403 mg/l. The iso-concentration contour map of chloride is shown in Figure 4.10. Chloride less than 250mg/l is shown in purple, Cl between 250 and 1000 mg/l is shown in blue, and Cl greater than 1000 mg/l is shown in yellow. Chloride is alarming in the area nearby Farah but within the acceptable limit in the north-western part and central area as well (fig 4.10).

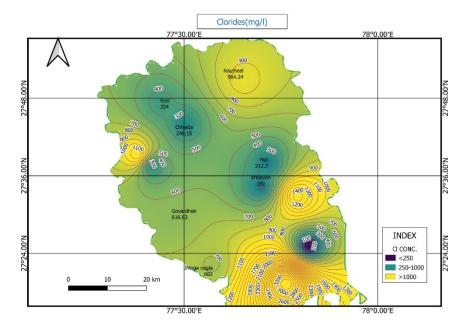


Figure 4.10 Iso-concentration map showing the spatial distribution of Chloride

4.11 pH

pH is one of the essential characteristics of water. Its desirable range is 6.5 to 8.5 as per BIS and WHO standards. It ranges from 7.66 to 8.43 with a mean value of 8.13, which falls within desirable limits in the study region. The spatial distribution of the pH values data is shown in Figure 4.11. The area that has a pH value greater than 8.5 is shown in yellow, purple represents the area where pH is below 6.5 and green shows the area where pH value is in the 6.5-8.5 range. The entire green area indicates that the pH is in an acceptable range in the Mathura district (fig 4.11).

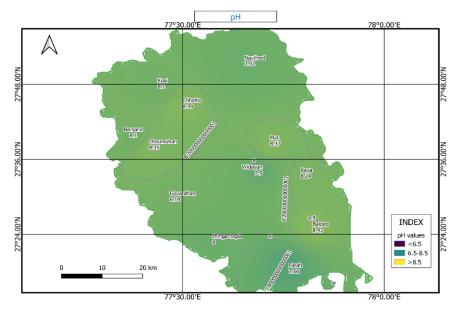


Figure 4.11 Iso-concentration map showing the spatial distribution of pH

4.12 Fluoride

Fluoride should be as low as possible. Its prescribed limit is 1 mg/l. High values of Fluoride causes fluorosis. It ranges from 0.07 to 6.53 mg/l with a mean value of 1.33 mg/l in the study zone. 50% of the samples are above the desirable value suggesting that the water is not suitable for drinking in those areas. The spatial distribution map of the F data is shown in Figure 4.12. F concentration less than 6 mg/l is shown in purple, the F range from 0.06 to 1.2 mg/l is shown in blue, the blue colour is used to show the area where F is between 1.3 and 1.5 mg/l and the yellow colour shows the area where the F concentration is above 1.5 mg / l. Figure 4.12 indicates that the F concentration in most of the areas in the district is above the desirable limit. Only three locations are shown in blue, suggesting that the F concentration in these areas is within desirable values.

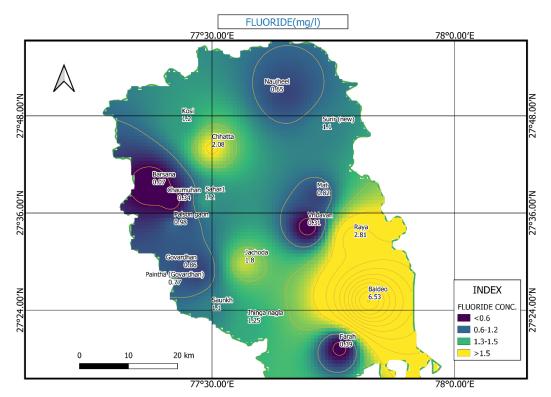


Figure 4.12 Iso-concentration map showing the spatial distribution of Fluoride

4.13 Correlation chart

Correlation chart is shown in figure 4.13. The Correlation chart shows that pH has high positive correlation coefficient with TH, TDS and negative correlation with EC only. TH is negatively correlated with EC only and has positive correlation coefficient with TDS, NO₃, Ca, Mg, and SO₄. EC is negatively correlated with all other parameters. TDS have

high positive correlation coefficient with Ca and NO₃. Mg and Ca are positively correlated with NO₃.

| | рН | TH | F | EC | TDS | NO3 | Cl | Са | Mg | Na | SO4 | НСО3 |
|------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|------|
| рН | 1 | | | | | | | | | | | |
| тн | 0.81226 | 1 | | | | | | | | | | |
| F | 0.527417 | 0.399821 | 1 | | | | | | | | | |
| EC | -0.78853 | -0.50206 | -0.25916 | 1 | | | | | | | | |
| TDS | 0.944922 | 0.926762 | 0.26777 | -0.65358 | 1 | | | | | | | |
| NO3 | 0.741478 | 0.986215 | 0.353971 | -0.45325 | 0.946333 | 1 | | | | | | |
| CI | 0.123844 | 0.064116 | 0.023703 | -0.03687 | -0.65959 | -0.03101 | 1 | | | | | |
| Са | 0.644691 | 0.915405 | 0.464727 | -0.38091 | 0.920978 | 0.906375 | 0.029805 | 1 | | | | |
| Mg | 0.707719 | 0.937348 | 0.502178 | -0.45054 | -0.0263 | 0.950543 | -0.02824 | 0.89256 | 1 | | | |
| Na | 0.151774 | 0.38069 | 0.23369 | -0.14631 | -0.34098 | 0.451976 | -0.26039 | 0.599631 | 0.546597 | 1 | | |
| SO4 | 0.478547 | 0.787788 | 0.243674 | -0.35357 | -0.00135 | 0.850448 | -0.25341 | 0.742169 | 0.873526 | 0.618875 | 1 | |
| НСО3 | 0.177925 | 0.273033 | -0.16045 | -0.13225 | -0.38819 | 0.312931 | -0.03352 | 0.000282 | 0.35475 | -0.13882 | 0.468665 | 1 |

Figure 4.13 Correlation chart

Chapter 5.

CONCLUSION

This study indicates that the knowledge of the basics of groundwater modelling, selection of the right numerical or analytical model and clear model objective will solve any problem related to contaminant transport in groundwater. The selection of appropriate models is governed by factors such as aquifer properties, hydrogeology, type of pollutants, and the solute transport process that occurs in one's study area.

Model calibration is also an important step in model development and it can be done manually or automatically. The finite difference method is used by MODFLOW-based software, while the finite element method is used by software like FEFLOW. No method is ideal, and each method has its own set of advantages and drawbacks. For numerically simulating contaminant transport in two dimensions, the mesh-free design is a sufficiently accurate and simple process. The outcomes of the EFGM and the evidence from the field investigation are quite similar.

- New methodologies, such as Arc Hydro Groundwater executable programming code and GIS CONTRAM, can be built by merging GIS and GMS.
- Analytical techniques with GIS and remote sensing approaches are used to locate appropriate groundwater locations for drinking and irrigation in the Mathura district.
- The findings suggest that majority of the water in the study area is unfit for drinking and irrigation.
- The suitable places determined based on geographical distribution features are in the Mathura district's north-east and south.
- Geogenic activity is the primary cause of elevated concentrations of many water quality indices.

Before using the water for drinking or irrigation, it is recommended that suitable treatment methods and measures should be implemented. Furthermore, to address the region's groundwater depletion, it is suggested that sprinkling irrigation be adopted for proper water resource utilisation and to avoid future water shortages.

REFERENCES

- Baalousha, H. (2009). Fundamentals of groundwater modelling. *Groundwater Modelling, Management and Contamination; Konig, LF, Weiss, JL, Eds*, 149-166.
- Baalousha, H., & Köngeter, J. (2006). Stochastic modelling and risk analysis of groundwater pollution using FORM coupled with automatic differentiation. *Advances in Water Resources*, 29(12), 1815–1832. https://doi.org/10.1016/j.advwatres.2006.01.006
- BIS 2012, Indian standard specifications for drinking water, B.S. 10500.
- Clement, T. (1997). A Modular Computer Code for Simulating Reactive Multi-Species Transport in 3-D Groundwater Systems. PNNL-11720. *Pacific Northwest National Laboratory, Richland, WA. 59 pp.*
- Dr. N J Shrimali, Daksh H Soni, M. A. M. (2019). A Study of Various Approaches for GroundwaterContaminant.http://iwwaahmedabad.org/images/downloads/papers/20 19/1913.pdf
- Elango, L. (2005). Numerical Simulation of Groundwater Flow and Solute Transport. *Allied Publishers Pvt. Ltd.pp.151-164. January 2005.*
- FEFLOW 7.3 Documentation Introduction. (n.d.). Retrieved June 30, 2021, from http://www.feflow.info/html/help73/feflow/01_Introduction/intro.htm
- Fouad, M., Hussein, E. E., & Jirka, B. (2018). Assessment of Numerical Groundwater Models. *International Journal of Scientific & Engineering Research*, 9(6), 951–974. http://www.ijser.org
- Harbaugh, A. W. (2005). The U.S. Geological Survey Modular Ground-Water Model the Ground-Water Flow Process. U.S. Geological Survey Techniques and Methods 6-A16, 253.
- Hem, J. D. (1985). Study and interpretation of the chemical characteristics of natural water. US Geological Survey Water-Supply Paper, 2254.
- Kipp, K. L. (1997). Guide to the revised heat and solute transport simulator: HST3D-Version 2. U.S. Geological Survey Water-Resources Investigations, 97–4157, 1– 158.
- Koukidou, I., & Panagopoulos, A. (2010). Bulletin of the Geological Society of Greece APPLICATION OF FEFLOW FOR THE SIMULATION OF GROUNDWATER FLOW AT THE TIRNAVOS (CENTRAL GREECE). 43(2010), 1747–1757.
- Krishna kumar, S., Logeshkumaran, A., Magesh, N. S., Godson, P. S., & Chandrasekar, N. (2015). Hydro-geochemistry and application of water quality index (WQI) for groundwater quality assessment, Anna Nagar, part of Chennai City, Tamil Nadu, India. *Applied Water Science*, 5(4), 335–343. https://doi.org/10.1007/s13201-014-0196-4
- Kumar, C. P. (2003). Introduction to Groundwater. *INTRODUCTION TO GROUNDWATER MODELLING* (Vol. 247667). http://nihroorkee.gov.in/sites/default/files/uploadfiles/CPK_GW_Modelling.pdf

- Kumar, C. P. (2012). Groundwater Modelling Software Capabilities and Limitations. *IOSR Journal of Environmental Science, Toxicology and Food Technology*, 1(2), 46–57. https://doi.org/10.9790/2402-0124657
- Mathura District Population Census 2011-2021, Uttar Pradesh literacy sex ratio and density. (2011). Retrieved July 24, 2021, from https://www.census2011.co.in/census/district/516-mathura.html
- Pinder G., G. W. (1978). Finite element simulation in surface and subsurface hydrology. Advances in Water Resources, 1(3), 175. https://doi.org/10.1016/0309-1708(78)90029-5
- Praveen Kumar, R., & Dodagoudar, G. R. (2009). Modelling of contaminant transport through landfill liners using EFGM. International Journal for Numerical and Analytical Methods in Geomechanics, 34(7), n/a-n/a. https://doi.org/10.1002/nag.817
- Sant Lal. (n.d.). DISTRICT BROCHURE OF MATHURA DISTRICT, U.P. Retrieved July 24, 2021, from http://cgwb.gov.in/District_Profile/UP/Mathura.pdf
- Souza, W.R., 1987, Documentation of geographical display program for the saturatedunsaturated transport (SUTRA) finite element simulation model: U.S. Geological water resources investgation report 84-9369 409 p.
- The, P., America, L., & World Health Organization. (1998). The world health report 1998 -- Life in the 21st century: A vision for all. *World Health Organisation*, 226. http://bases.bireme.br/cgibin/wxislind.exe/iah/online/?IsisScript=iah/iah.xis&src=google&base=PAHO&lan g=p&nextAction=lnk&exprSearch=25006&indexSearch=ID
- Vyas, A., & Jethoo, A. S. (2015). Diversification in Measurement Methods for Determination of Irrigation Water Quality Parameters. *Aquatic Procedia*, 4(Icwrcoe), 1220–1226. https://doi.org/10.1016/j.aqpro.2015.02.155
- Wang, D., Wu, C., Huang, W., & Zhang, Y. (2019). Vibration investigation on fluidstructure interaction of AP1000 shield building subjected to multi earthquake excitations. Annals of Nuclear Energy, 126, 312–329. https://doi.org/10.1016/j.anucene.2018.11.021
- WHO. (2008). Guidelines for Drinking-water Quality THIRD EDITION INCORPORATING THE FIRST AND SECOND ADDENDA Volume 1 Recommendations Geneva 2008. WHO Library Cataloguing-in-Publication Data.
- Zheng, C., & Wang, P. (1998). MT3DMS: A modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems. US Army Corps of Engineers Engineer Research and Development Center, June, 239. http://www.geo.tufreiberg.de/hydro/vorl_portal/gw-modellierung/MT3DMS Ref Manual.pdf

VITAE

| | Authors | Specialization |
|----------------------|---|----------------------------|
| Per San | Mr. Manoj Kumar | Environmental Engineering |
| | M.Tech Scholar | Civil Engineering |
| | Deptt. Of Environmental Engineering, | |
| | Delhi Technological University, Delhi – | |
| | 110042 | |
| In the second second | E-mail - | |
| | Mr. Anunay A. Gour | Environmental Engineering, |
| | Assistant Professor, | Civil Engineering, |
| (o o l | Deptt. Of Environmental Engineering, | Environmental Impact |
| | Delhi Technological University, Delhi – | Assessment & Audit, |
| | 110042 | Industrial Waste |
| | E-mail – anunaygour@dtu.ac.in | Management |