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Abstract: In India, groundwater is a primary source of freshwater and used mainly for agriculture and irrigation purposes. Approximately 80% of the population is dependent on groundwater for household and agricultural purposes in India. The pace of urbanization in Gandhinagar has been accelerated since the capital of Gujarat state was formed; hence a study is carried out to identify the status of groundwater quality in the Chhatral area of Gandhinagar city. In this study, MODFLOW and MT3DMS software are used to identify contaminated groundwater status in particular study areas. MODFLOW software helped in simulating ground water quality under various hydro-geological conditions. After the initial simulation, the area was assigned to MT3DMS, a three-dimensional multi-species solute transport model where arsenic and fluoride concentrated chemicals are figured out above the permissible limit authorized by WHO and BIS for drinking purposes. The results of this study demonstrated that there is need to take necessary steps to control ground water quality in the study area. Groundwater quality modelling will help the stakeholders, government organizations & users to get the exact groundwater quality status for future use.

Keywords: Groundwater contamination, Arsenic, Fluoride, MODFLOW, and MT3DMS

I. INTRODUCTION

Groundwater is the most valuable and geographically scattered resource on the planet, and it is replenished annually through periodic precipitation. Groundwater is being used for drinking, irrigation, and industrial purposes. However, groundwater resources are under stress as a result of population increase, urbanization, and farming activities. In certain sections of the nation, growing water demands have resulted in groundwater extraction reaching yearly replenishment because urbanization changes occur due to a decrease of recharge with an increase in withdrawals. In India, approximately, 62% of the groundwater is used for irrigation, 85% is used in rural water supply and 50% in urban water supply according to the central groundwater board dynamic groundwater report - 2021.

The national water policy of 2012 has emphasized the scientific assessment of groundwater resources. In India, the average annual rainfall is 1283 BCM, with a net groundwater availability of 411 BCM and net annual groundwater availability is 396 BCM, whereas the annual groundwater draft for irrigation, domestic and Industrial is 243 billion cubic meters and the stage of Groundwater Development for the country as a whole is 61%. (Board, 2019) Safe drinking water is a prerequisite for development since it is necessary for agricultural production, public health, industrial development, economic development, and sustainable livelihoods. (Zhang) However, rising population, urbanization, and industry pose a threat to water quality management by altering consumption patterns and lowering quality. (Poonam Tirkey, 2017)

In the Ground Water Resources Assessment-2017 report, the Central Groundwater Board (C.G.W.B) categorized Gandhinagar and Mehsana as over-exploited areas. Excessive development in industrial areas can cause water to be contaminated with an enormous amount of highly concentrated chemicals as a waste product of industries and, subsequently, decrease the physical and chemical properties of groundwater.

The objective of this study is to develop the numerical model using MODFLOW and MT3DMS for solute transport & to identify the contamination process of the groundwater from polluted drains in the study area.



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II. GROUNDWATER MODELLING

Model is used for a better understanding of the resources and their functioning in response to the environmental and man-made changes in the system. The finite element and finite difference model are a type of gridded method where it solves the mathematical equations at each specified grid cell and integrate using mass conservation principle across the boundaries examples of such tools include MODFLOW, PLASM, FEFLOW, SUTRA, MT3D, and SEAWAT (Singh, 2016).

A model is a simplified representation of a real system and the processes occurring within it that approximates the system's excitation-response relationships which are of interest_(Kavalanekar, 1992). Basically, in the groundwater model, various numerical solution techniques were used to predict the various effects of hydrological and hydrogeological changes in the aquifer, to stimulate and describe real-world groundwater flow, and also been used to predict future aquifer response. There is a wide range of groundwater modeling programs out there already, each with its own set of capabilities, operational characteristics, and constraints. If modeling is being considered for a project, it is critical to evaluate whether a certain code is acceptable for the project or if a code that can conduct the simulations needed in order serves a purpose. _(Kumar, Groundwater Modelling Software – Capabilities and Limitations, 2012) Here are various groundwater models used for studying groundwater systems to stimulate the flow of groundwater with different case studies.

MODFLOW represents the United States Geological Survey's modular finite-difference flow model, a computer program that solves the groundwater flow equation. Hydrogeologists use the application to simulate the flow of groundwater through aquifers. MODFLOW model is developed to estimate the head calibration of a part of the Mahesh River basin with the known boundary conditions and field observations. (Khadri, 2016)

MT3DMS is used to stimulate alteration in groundwater concentration of harmful contaminants with considering features like advection. Dispersion and diffusion and other basic chemical reaction within various types of boundary conditions and sink and source mixing package. Multiple transport solution techniques were included in the MT3DMS, which can apply to a wide range of contexts, including model calibration (Banejad). A case study was conducted in Al Batinah coastal plain, Sultanate of Oman with MODFLOW and Mt3DMS, to study the transient groundwater flow and solute transportation process and focus on two criteria artificial groundwater recharge by using desalinated water and reduction in groundwater abstraction. (Chitrakar, 2016)

PM-WIN: Processing MODFLOW for windows.PM-WIN is one of the most complete groundwater simulation systems in the world. This Supports models such as MODFLOW, MT3D, MT3DMS, MOC3D, PEST2000, and, VCODE. PMWIN has an advanced and powerful graphical user interface, as well as supporting models and programs and a combination of multiple modeling tools. (Kumar, Groundwater Flow Models; Chiang). A case study of Rafsanjan aquifers concluded that PMWIN software is the best-suited alternative for the simulation of an unconfined layer of the aquifer with its water quality and quantity of groundwater. (Rahnama, 2013)

Other models are including of DRASTIC model where seven risk indexes are taken into consideration as in one layer in the model. Where, D shows the depth of the aquifer, R shows Recharge, A shows Aquifer media, S shows Soil media, T indicates Topography, I is the Impact of the Vadose zone and C shows Hydraulic conductivity by using the Analytical hierarchy process and fuzzy logic. (Zhang)

Visual MODFLOW uses MODFLOW-2000, MODPATH, MT3DMS, and RT3D to deliver professional 3D groundwater flow and pollutant transport modeling. Visual MODFLOW Pro is the most extensive and sophisticated graphical modeling environment available, combining the regular Visual MODFLOW software with Win PEST and the Visual MODFLOW 3D-Explorer. Run the simulations for groundwater flow, path line, and pollutant transfer. Using Win PEST or manual approaches, calibrate the model automatically. (Vishwakarma)

III. STUDY AREA

Gujarat is located between 20° 06' 00" and 24° 42' 00" north latitude and 68° 10' 00" to 74° 28' 00" east longitude. Gujarat has the country's longest coastline, stretching over 1600 kilometers. It runs from Lakhpat in the north to Daman in the south. Rajasthan, Madhya Pradesh, and Maharashtra have shared borders with the state, as well as an international border with Pakistan in the northwest. Gujarat has 18,225 villages and 348 towns, with 16 of them having a population of over a million people. There are 60,383,628 people in the city, with 31,482,282 men and 28,901,349 women according to 2011 census.[14] The geographical area of Mehsana taluka is 770.81 sq. km. Basin/Sub-basin considered as Rupen/Saraswati and Principal Aquifer system is Quaternary, Alluvium Major Aquifer System is Older & Younger Alluvium and Normal Annual Rainfall is 785 mm[15]. The study area map is shown in figure(i) which consists of a map of India and further into Gandhinagar, Mehsana, Kadi, and Kalol areas of Gujarat state. Moreover, the distribution of the area is in Gandhinagar, Kadi, Kalol, and Mehsana which is stated as an Over-exploited area of Gujarat by the Central Groundwater Broad assessment report-2017.



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A. Topography

Geographical area of Mehsana taluka is 770.81 sq. km. Basin/Sub-basin considered as Rupen/Saraswati and Principal Aquifer system is Quaternary, Alluvium Major Aquifer System is Older & Younger Alluvium and Normal Annual Rainfall is 785 mm and the area is almost flat covered by alluvial soil and the slope in major part of the Mehsana region ranges from 0 to 1% that is almost flat. (Prakash, 2015)

B. Climatic Condition

Droughts are frequent in north Gujarat, Saurashtra, and Kachchh regions due to poor and erratic rainfall. The climate varies from humid in the south through sub-humid in the central part to semi-arid and arid in the northern and western parts. The state receives rainfall mainly during the southwest monsoon period.

C. Hydrogeological Features

Proper characterization of the hydrogeological conditions at a site is necessary to understand the importance of relevant flow or solute transport processes. Without proper site characterization, it is not possible to select an appropriate model or develop a reliably calibrated model. (Kumar, Groundwater Modelling Software – Capabilities and Limitations, 2012)

IV. DATA COLLECTION

The collection of the data is another important aspect of the simulation of the model. In the present study area. Data are collected from Central Groundwater Board(C.G.W.B) and Gujarat Water Resource Development Corporation Ltd.(G.W.R.D.C). The data consist of well data, the concentration of fluoride, Physical contaminates like Electrical Conductivity and TDS, Transmissivity. After a thorough study of existing and current data and reports by C.G.W.B, it was shown that this area has a high amount of toxicity in groundwater due to the nearby industrial areas. The industrial area is defined in the figure with the help of the OSM plugin in QGIS. The Chhatral region of Gandhinagar and Mehsana is an industrial region of Gujarat, as seen in fig. 2.



Figure 1 Industrial Area



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The concentration of total dissolved solids and EC is varying due to the presence of salt and other harmful minerals. Firstly, from the TDS and EC values it can be justified that the presence of minerals and values ranging from 790-8470 mg/L and 1500-18000 μ S/cm respectively, are above the permissible limit measured for drinking purposes as per BIS standards. The permissible limit of TDS and EC should be below 2000 mg/L for drinking purposes. (Standards, 2012). The graph shows the value of Total Dissolved Solids from the year 2017 to 2021 and EC is given by CGWB and GWRDC accordingly in fig. 4 and fig. 3 respectively. The graph indicates that the maximum wells have TDS above the permissible limit and increasingly from 2017 to the 2021 year.

The pan type digital EC and TDS meter is used to measure TDS and EC in situ. Dissolved ionized solids are directly proportional to the electrical conductivity of the water. Ions from dissolved particles in water cause the current to conduct an electric current, which may be measured with a standard conductivity or TDS meter. Ions from dissolved particles in water cause the current to conduct an electric current, which may be measured with a standard conductivity or TDS meter. (Kavindra J, 2020) Diseases like Cancers, melanosis, hyperkeratosis, peripheral, vascular disease, gangrene, molting teeth, weakening of bones, arthritis, and neurological damage are all effects of excessive value of fluoride and arsenic in groundwater.



Figure 2 Total Dissolved Solid of wells in Study area



Figure 3 Electrical Conductivity of study area

In the concerned study area, the maximum concentration of fluoride and arsenic is 2.96 mg/L and 0.03 mg/L respectively from the Mehsana district as per the given data, the concentration value is exceeded the permissible limit recommended by WHO for fluoride and arsenic is1.5 mg/L, and 0.01 mg/L respectively. Around 1,22,000 people live in Gujarat state where arsenic concentration is exceeding from 0.01 mg/L and out of which 49,000 people have consumed water from groundwater with having a high amount of arsenic concentration. (Polya, 2021)



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V. METHODOLOGY

Groundwater modelling is a tool that can assist in the investigation of groundwater challenges. Many hydrologists, geologists, engineers, and other researchers rely on numerical-based groundwater tools. A variety of software applications were used to analyze groundwater. A model is a simplified representation of a real-world system, and the first stage is to create a conceptual model. It is made up of a collection of assumptions that represent the compositions of real-world systems, their transport mechanisms, the main processes that regulate them, and the relevant medium qualities.

VI. QGIS

QGIS is a free and open-source platform for geographic Information systems which acknowledge individuals to analyze and survey spatial information with a graphical representation of data and create and generate maps of different spatial data. This software supports raster, vector, and mesh layer files.

A tile of a specified area is downloaded from various sites like Bhuvan.nrsc, Earth Explorer by U.S.G.S, etc. Wherein, raster format with .tiff extension. The tiff file is digitized and imported into the raster layer in QGIS. In addition to well data from the State water data center, wells are assigned in Gandhinagar, Mehsana, Kadi, and Kalol areas by given Latitudes and longitudes with the well points. Besides, Wells are added in Delimited Text layer from the layer tab by importing values of latitude and longitude with identifying names of the well along with an appropriate projection of the study area as shown in fig. 5. The contours are formed from the DEM file in raster format as shown in fig. 6.



Figure 4 Well Location in Study Area

Figure 5 Contours of Study Area

VII. MODFLOW

MODFLOW 6 adds additional metadata of the discretization approach not present in previous MODFLOW versions (Langevin, 2017). MODFLOW is selected as the model for the groundwater flow and prediction of groundwater contamination in the Chhatral region and area surrounded by aquifers in Gandhinagar, Mehsana, Kadi, and Kalol. The model simulates groundwater flow over an area of 2750 Sq.km with 7 columns and 7 rows with a single vertical layer. MODFLOW 2005 can stimulate the aquifers layer type that can be confined, unconfined, or a combination of the layers. On the contrary, MODFLOW 6 can only consider a confined layer by default and also stimulate both steady and transient flow in the irregular-shaped flow of groundwater. 0 to 1 year is taken into consideration as a steady flow and from 1-2 years as a transient flow. The units of the model are set as in meter and second.

The very first step of analyzing the groundwater flow model is creating and importing the study area, which was created in QGIS and assigned to the model domain with an appropriate extension. From QGIS, the shapefile of the study area is imported into the model with no grid option. The model domain is discretized with 3 layers in the z-direction as a Model top, Upper aquifer, middle aquifer ad lower aquifer. The gride cell dimension of the study area is 0.1*0.1 as shown in fig. 7. The number of Z formula adopted as two as higher z value is assigned to model top and lower Z value as a lower aquifer. The data collected from the C.G.W.B were added up to the grid of the study area that includes the thickness of aquifers are 100m,-150m,-210m, and -300m for the model top, upper aquifer, middle aquifer, and lower aquifer respectively. Furthermore, the deliberate upper aquifer layer is an unconfined aquifer as a convertible layer from MODFLOW 2005.





The governing mathematical equations of the groundwater flow are derived by a mathematical combination between the water balance equation and Darcy's law. The groundwater flow can be described in 3D under non-equilibrium conditions in a heterogeneous and anisotropic medium using the following equation an also a general form of governing equation used in MOFLOW that describes the three-dimensional movement of groundwater flow of constant density through porous media is, (Rushton, 2003)

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$$\frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right) \pm W = S_s \frac{\partial h}{\partial t}$$

Where, K_x, K_y, K_z are hydraulic conductivity along with x, y, and z-direction,

h = piezometric head(L),

W = Volume flux per unit volume,

S = specific storage or specific yield and,

t = time(T).

The fluxes in the three coordinate directions are represented on the left side of the equation, while the storage contribution following the change in groundwater head over time is shown on the right side.

The Constant Head boundary condition is used to keep the head value constant in specified grid cells regardless of the system parameters in the surrounding grid cells, effectively functioning as an infinite source of water entering the system or an infinite sink of water exiting the system. The Well Package(WEL) is meant to enhance features including wells that extract or add water to the aquifer at a predetermined rate during a stress period, with the rate being independent of both the cell area and the head in the cell (Langevin, 2017). The well points are assigned to the model with a specified grid cell size in the study area. The shapefile of well points from QGIS import with the extension of .shp with a separate object as shown in figure(ix); the rhombus shape indicates the well in the study area. There is total 15 wells are assigned to the study area with their latitude, longitude, and piezometric level assumed as a water elevation. The well packages from MODFLOW packages and program are implemented and all wells with the corresponding cells are assigned and relocated into well packages with assumed pumping rates. The General-Head Boundary (GHB) Package simulates flow from an external source into or out of a cell (n) in accordance with the difference between the head in the cell and the head allocated to the external source. The proportionality constant was used, as a boundary conductance. the value of the conductance is 0.01 for the steady period and 0.002 for the transient period. The drain package is for modeling the consequences of groundwater, which extract groundwater from the aquifer at a rate that is proportional to the difference between the aquifer head and the head of the assigned drain. Although, the recharge of the drain is to be zero. (Chiang). A recharge package(RCH) is anticipated to the model over an area recharge is distributed to the groundwater system. Here, in the Chhatral region as a study area, the whole region is taken into the recharge area with the help of the polygon tool as shown in fig.8. Aquifer recharge is most commonly caused by precipitation that percolates into the groundwater sources.



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VIII. MT3DMS

Multiple Transport Techniques were there in MT3DMS with the inclusion of finite difference method(FDM), modified Method of Characteristics (MOC) Modified Method of Characteristics (MMOC) for particle tracking as a mixed Eulerian-Lagrange method, and third-order variation diminishing(TVD) packages with mass conservation while limiting mathematical dispersion and artificial oscillation. (C. Zheng, 2013). The concentration of arsenic and fluoride was simulated with the MT3DMS code. The model with the grid is assigned with MT3DMS packages after the completion of the MODFLOW program. The model with zero discrepancies is followed by the MT3DMS, the model with zero discrepancy as shown in fig. 9, where different packages are involved, like Basic Transport Model, Advection-Dispersion Model, Sink and Source model, and Generalized Conjugate Gradient solvers.



Figure 7 Drainage Package



Figure 8 Discrepancy rate



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The partial differential equation describing the fate and transport of contaminants of species k in three-dimensional, transient groundwater flow systems can be written as follows (Wang):

$$\frac{\partial(\theta C^{k})}{\partial t} = \frac{\partial}{\partial x_{i}} \left(\theta D_{ij} \frac{\partial C^{k}}{\partial x_{j}} \right) - \frac{\partial}{\partial x_{i}} (\theta v_{i} C^{k}) + q_{s} C_{s}^{k} + \sum R_{n}$$

Where, C_k is the concentration of dissolved species $k(ML^{-3})$, θ is the porosity of subsurface, t is time, x_i is distance concerning cartesian coordinate (L), D_{ij} is the hydrodynamic dispersion (L^2T^{-1}) , v_i is seepage velocity(LT^{-1}), q_s is a volumetric flux of aquifer showing fluid source as a positive and sink as a negative(T^{-1}), C_s^k is the source or sink flux concentration for k species(ML^{-3}), ΣR_n is chemical reaction term($ML^{-3}T^{-1}$).

IX. CALIBRATION

A model calibrated to a set of conditions that are not representative of actual field conditions may emerge from a lack of available exposure assessment. To specify hydraulic conductivity, storage coefficient, dispersive, and porosity in groundwater flow and transport modeling using MODFLOW and MT3DMS, probably calibrated parameters are needed. A trial-and-error technique has been used to calibrate the model by modifying the parameters like recharge rate, pumping rate, hydraulic conductivity, and changing the step size.

X. RESULTS

The simulation model of MT3DMS shows the transport of concentration of arsenic and fluoride from the source of concentration to the entire study area within 1-2 years. The concentration of fluoride with the contours shows in fig.10, which simulate the dispersion of fluoride concentrations were measured locations over. The concentration of arsenic in specific areas throughout the area of research is visualized in Fig 11. The result indicates the value of arsenic and fluoride in the chhatral region by using wells in surrounding areas.

In the evaluation of the quality parameters existing in groundwater, it was observed that some parameters such as fluoride, arsenic, EC, and TDS have a trend to increase during the next

years in a particular area, with in

creasing industrial activities.



Figure 9 Fluoride Concentration





XI. CONCLUSION

Remote towns with inadequate water supply systems lead to a higher risk of long-term geogenic and anthropogenic contaminations., frequently, due to not evaluating groundwater for chemical contamination on yearly basis or might be due to local and national government's lack of expertise and resources to address the issues. It is notified that the values from the data, are potentially at high risk and make the surrounding area contaminated.

This study reveals that MODFLOW and MT3DMS is a suitable options for the simulation of groundwater flow and contaminate transport models for unconfined aquifers. The concentration of arsenic and fluoride is only considered in upper aquifers because of the piezometric head and near to the subsurface of the ground. The values of considered chemical and physical parameters are fluoride and arsenic, and Electrical conductivity and TDS respectively, are hazardous for drinking and agricultural purposes.

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