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Application of Conceptual model in contaminant transport phenomena: Case study of a region between Bharaj and Orsang rivers of Gujarat, India

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Abstract*— The anatomy of groundwater for drinking purpose can easily be understood by considering its quality and contamination. IS 10500-2012 specifies the general and physical groundwater quality parameters. This study has focused on modeling aspect of contaminant hydrology where an attempt has been made to model a groundwater flow and contamination transport model for the region between Bharaj and Orsang rivers of Gujarat. Primary input model parameters for the groundwater flow model are average annual recharge (m/d), digital elevation of the site being model (m), water table (m) in observation wells, lithology, aquifer characteristics such as thickness (m), transmissibility (m^2/d), hydraulic conductivity (m/d), and specific yield of aquifer material. A two dimensional conceptual model for the site has been developed using basic MODFLOW-2000 package in Groundwater Modeling System. After submitting required input data, conceptual model is converted to finite difference grid based numerical model. Various simulations performed for the groundwater flow model evaluated the suitability of study area with respect to potential groundwater contamination. The results obtained from MODFLOW model will be used as the flow field for a transport simulation in MT3DMS model. An MT3DMS- conceptual transport model involving advection-dispersion packages assumed for the worst case scenario has been adopted. Final outcome of the transport model gives a time series plot explaining the long term potential for migration of contaminants present in study area.

***Keywords*— Contamination, Groundwater, MODFLOW, MT3DMS, Transport**

I. INTRODUCTION

Important stages involved in the development of a transport model explained by (Anderson Mary, 1992) are Conceptual model design, Development of physical/mathematical model, Model calibration, Sensitivity analysis and Future prediction. A groundwater flow model describing water level contours and flow in and out of the system is developed by two different methods. First one being a grid approach where a finite difference grid is created and input parameters entered in cell by cell basis.

Generally, grid approached being a simple method for small scaled areas, is preferred for example problems in academics. Second approach is of a Conceptual model using regional and site-specific hydro-geologic and climatic information as derived from the field observations. (He, 2004) The conceptual model is generally developed with various coverages such as boundary, source/sinks, recharge, aquifer layers and an observation well coverage for calibration of the model.

Conceptualised contamination transport models can specifically simulate the origin of contaminant and its release in the subsurface medium. (Morrison, 2014) Groundwater contamination, as per WHO usage (UNESCO, 1992) is: Introduction into water of any substance in undesirable concentration not normally present in water, e.g. microorganisms, chemicals, waste or sewage, which renders the water unfit for its intended use'. The term groundwater pollution is defined in the International glossary of hydrology (UNESCO, 1992) as: 'Addition of substances which impair the suitability of water for a considered purpose'. (Zaporozec, 2002)

MT3DMS is a three dimensional modular-transport model in a two-step Flow and Transport simulations used in conjunction with MODFLOW. After the calibration of Flow field, the contaminant source locations, species and their concentration values are defined into the model. The advection-dispersion and diffusion chemical reactions are involved in MT3DMS. It is developed by (Chunmiao Zheng, 1990) using Finite Difference Method. The rate of solute transport in advection process is usually equal to average seepage velocity by the surging fluid in reaction to a hydraulic gradient. (Mohamed, 2018)

Diffusion process is molecular-based where the transport takes place from high to low molecular concentration. It is governed by the continuous change in various parameters such as thermal gradient and pressure gradient. The dispersion process is associated with the spreading nature of fluid particles that are at one time close together tend to move apart due to variations in the velocity and movement in the porous medium of the fluid. (Mohamed, 2018)

A significant database useful as input parameters is adopted while developing conceptual model since they attend to site-specific conditions. Source/sinks coverage alone requires details on rivers, drains, wells and other specified head boundaries. Present study focused on building a flow field using above mentioned coverages in MODFLOW 2000 (Harbaugh et al.,2000). Based on groundwater quality reports of GWRDC (Ground Water Resources Development Corporation) and NRDWP (National Rural Drinking Water Programme), Nitrate (mg/l) has been considered in contaminant transport model. GMS- Groundwater Modeling System software has been used to perform simulations as it is a widely adopted tool.

II. STUDY AREA AND DATA EXPLORATION

The study area is comprised of two talukas of Chhota Udepur district namely Jetpur Pavi and Chhota Udepur. Bharaj river originating from sukhi reservoir moving south west direction and Orsang river a tributary of Narmada river, originating from the state of Madhya Pradesh and joining each other at 22.3226 latitude and 73.8196 longitude. The highest elevation of the site being modeled is 150m and lowest being 90m above mean sea level occupying 61.57 km^2 area having mean slope surface less than 2% in south west direction.

Average annual rainfall for the terrain is 1119 mm and normal monsoon rainfall is 1097 mm per year. Maximum-recorded temperature is 45°C and minimum of 7°C with very wide seasonal temperature variations Land use map developed from Landsat images shows high agricultural activities and low barren lands for study region. Chhota Udepur Taluka consists of 27,687 hector area of forest and 5324 hector of barren land. (P.L.SHAH, 2016-2017)

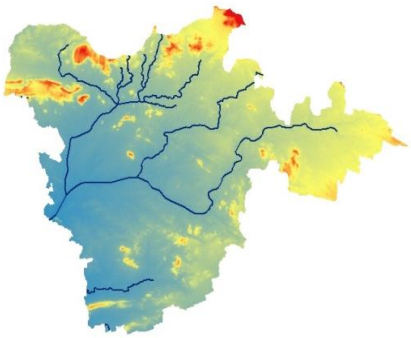


Fig.1: Elevation Model of Study Area

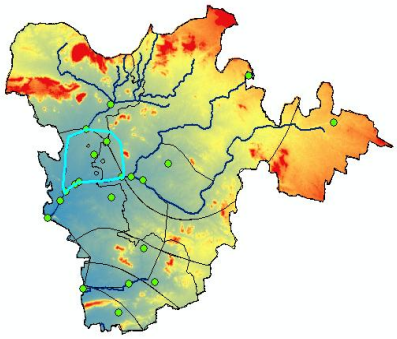


Fig.2: Contamination Site Locations



Fig.3: World image of Site location

Data collection and exploration related to site has been mentioned in a table below with respect to different government bodies and reports published by them. Integration of various data sources such as groundwater level, groundwater quality and SRTM digital elevation model pointed towards a potential contamination site seen in figure 3. After screening data related to groundwater quality, it was found that Nitrate concentrations excides permissible limits (more than 45 mg/l) for drinking water provided by IS 10500-2012 for few of the shallow tubewell sources present in the region, highest being 261 mg/l.

Lithology data is useful when a solid conceptual model development is required, different zones trapped in lithology is assigned with different horizontal hydraulic conductivities as well as horizontal and vertical anisotropies. From groundwater level data is observed in the range of 6.6 to 15.6 m for pre monsoon period and 2.3 to 11.6 m in post monsoon season denoting a significant recharge.

Table. 1: Data Sources Exploration

Data Type	Government Body	Remarks
Precipitation	SWDC, Gandhinagar	Last 30 year time period
Lithology	GWRDC, Gandhinagar	Hard Basalt zone
Groundwater Quality	GWRDC, Gandhinagar	-
Groundwater Quality	Reports of CGWB & NRDWP	High Nitrate & Fluoride

III. MATERIALS AND METHODOLOGY

Groundwater flow and contaminant transport problems are easily solved using Numerical models. GMS is a concept based advanced system that allows performing simulations for different methods such analytical and numerical. A standard step wise modeling process described by (Anderson Mary, 1992) is adopted for present research work.

1. Data Collection
2. Conceptual Model construction
    a. Coverage set up
    b. Assigning packages
3. Multi-dimensional Grid Creation
    a. Finite Difference Grid
    b. Assign cell values
    c. Interpolate cell values
4. Initialize MODFLOW
    a. Check Simulation
    b. Fixing Errors
5. Run MODFLOW
    a. Simulate flow field
6. Reading Solution and Flow Budget
7. Initialize MT3DMS
    a. Define Contaminants and Concentrations
    b. Define Packages
    c. Set Stress period
8. Run MT3DMS
9. Read Solutions

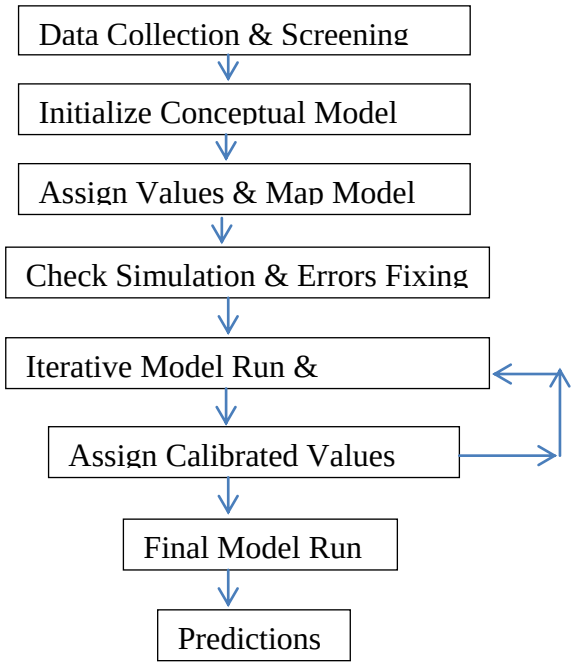


Fig.4: Modeling process Flow Chart

Governing Equations:
For the groundwater flow model: The partial differential equations, describing the groundwater flow, velocity and contaminant transport, can be expressed as follows (Harbaugh(2005), Zheng and Wang(1998))

$$\frac{\partial}{\partial x}\left[k_x\,\varphi\,\frac{\partial \varphi}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_y\,\varphi\,\frac{\partial \varphi}{\partial y}\right]+\frac{\partial}{\partial z}\left[k_z\,\varphi\,\frac{\partial \varphi}{\partial z}\right]=\left[\frac{\theta}{\eta}S_s+C(\varphi)\right]\frac{\partial \varphi}{\partial t}\pm Q$$

For the contaminant transport model:

$$\frac{\partial}{\partial x}\left[\theta D_{xx}\frac{\partial c}{\partial x}+\theta D_{xy}\frac{\partial c}{\partial y}+\theta D_{xz}\frac{\partial c}{\partial z}\right]+\frac{\partial}{\partial y}\left[\theta D_{yx}\frac{\partial c}{\partial x}+\theta D_{yy}\frac{\partial c}{\partial y}+\theta D_{yz}\frac{\partial c}{\partial z}\right]$$
$$+\frac{\partial}{\partial z}\left[\theta D_{zx}\frac{\partial c}{\partial x}+\theta D_{zy}\frac{\partial c}{\partial y}+\theta D_{zz}\frac{\partial c}{\partial z}\right]-\left[\frac{\partial}{\partial x}(v_x C)+\frac{\partial}{\partial y}(v_y C)+\frac{\partial}{\partial z}(v_z C)\right]$$
$$=\frac{\partial}{\partial t}(\theta C)+\rho_b\frac{\partial s}{\partial t}+K_m\theta C^m\pm R$$

Where,
x, y, z are the Cartesian coordinate axes; t is time in days;
kx, ky, kz are the hydraulic conductivity along the respective Cartesian x, y, and z coordinate axes;
φ is the pressure head;
θ is the moisture content;
η is the effective porosity of the porous media;
Ss is the specific storage of the porous media;
$C(\varphi)$is the specific moisture capacity;
Q is a volumetric flux per unit volume representing sources and sinks of water;
C is the concentration of contaminants dissolved in groundwater
(Source: Chen C C, 2016)

IV. APPLICATION OF CONCEPTUAL MODEL

For present research work, a Conceptual model "Concept_T1" was developed with various coverages such as Boundary, Rivers, Drains, Aquifer Layers, Recharge, Wells and Observation Wells. Boundary coverage as the name suggest was assigned a polygon defining boundary of the site. In River coverage, first rivers were created using map module and creating arc toolbox, a general head boundary was assigned to rivers. River nodes were denoted with elevation values from SRTM digital elevation model where values vary linearly along the arcs.

Drain coverage was setup defining creek beds existing in the region and same as River coverage, elevation values was assigned from elevation raster. Wells coverage contains a few wells present in the study region denoting flow rates in cubic meter per day. Recharge and Aquifer coverages are important as the recharge rate and hydraulic conductivity drives the flow model. Recharge rate in meter per day was computed using various methods such as Rainfall infiltration factor method, Water Level Fluctuation method and some of the empirical formulas as well. Percentage deviance from these methods helped in determining recharge of 0.00026 meter per day.

Aquifer coverages are introduced based on lithology and zones trapped while exploring a bore well. In current study layer 1 is a fine to medium weathered materials and layer 2 is a hard basaltic zone. Representative values of hydraulic conductivity has been assigned to these aquifer layers and then calibrated to get accurate results. Another ways to introduce conductivity is to develop a stratigraphy model and generate data from solids, different elevation rasters can also be used to create solids.

Model calibration has been performed considering observation wells present in study region. Computed groundwater head and observed groundwater heads are compared in different simulations to reduce error present in observation head interval, which is kept 1.5 meter for the region. After all the coverages are set up, a finite difference grid gas been created for the cell sizes of 60 meter in both X and Y direction, also for Z direction number of cell is 2 and a constant bottom cell elevation is adopted. Thus, a map module based conceptual model is converted to grid based numerical model to simulate various computations.



Fig.5: Aquifer layer 1 Coverage



Fig.6: Observation Wells Coverage

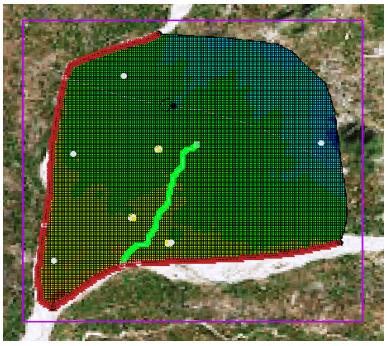


Fig.7: Conceptual to Numerical Grid

Table. 2: Input Model Parameters

Parameter	Value	Unit	Remarks
Recharge	0.00026	m/d	Computed
Hydraulic Conductivity	10.0 to 60.0	m/d	Calibrated
Porosity	0.3		Calibrated
Layer 1 Top Elevation	SRTM Elevation Raster	meter	Interpolated
Layer 2 Bottom Elevation	80	meter	Constant
Layer 2 Bottom Elevation	50	meter	Constant
Vertical Anisotropy	4	m/d	Calibrated
Wells	20-610	m^3/d	extraction
Observation wells	5.0 to 8.0	mbgl	observed
Nitrate Concentration	190-262	mg/l	observed
Longitudinal Dispersivity	12.4	meter	Computed

V. RESULT ANALYSIS AND DISCUSSION

After successful termination of steady state type MODFLOW, simulation result is obtained showing plan and front view in figure 8 and 10 respectively. Simulated groundwater level is in the range of 91.5 to 111.5 meters along the raster

elevation. The direction of the flow is south-west, same as observed from observation wells. Cells selected in the vicinity of the wells shows a cone of depression indication flow out of the system.

Flow Budget from final MODFLOW simulation suggests that flow (m3/d) into the system 19307.47 is higher than flow out of the system 11126.45 by sources and sinks indicating sufficient normal rainfall recharge. Total zone flow into the system is 5223.45 and 13404.41out of the system. Thus, total flow in and out of the system having 0.00022 percentage difference indicates a need of managed aquifer recharge.

A steady state MT3DMS simulation is performed with maximum Nitrate concentration of 225 mg/l for a single stress period of 20 years. Values of nitrate concentration are from data explored in NRDWP reports for the financial year 2017-2018. Assuming the worst case scenario, only Advection and dispersion packages are turned on. The transport observation package is also applied which determines mass flux into sources and sinks. Transport simulation results in to spread of nitrate in the direction of groundwater level towards the extraction wells for 20 year time step.

More précised results can be obtained while trying alternate packages and comparison between simulations, Error vs. Simulation and Error vs. Time step plots can also improve final outcome. A separate groundwater evaporation and transpiration package can be adopted rather than incorporating it in recharge package. An active dataset time series plot can be used to understand linear relation between mass influx and time for a particular cell location.

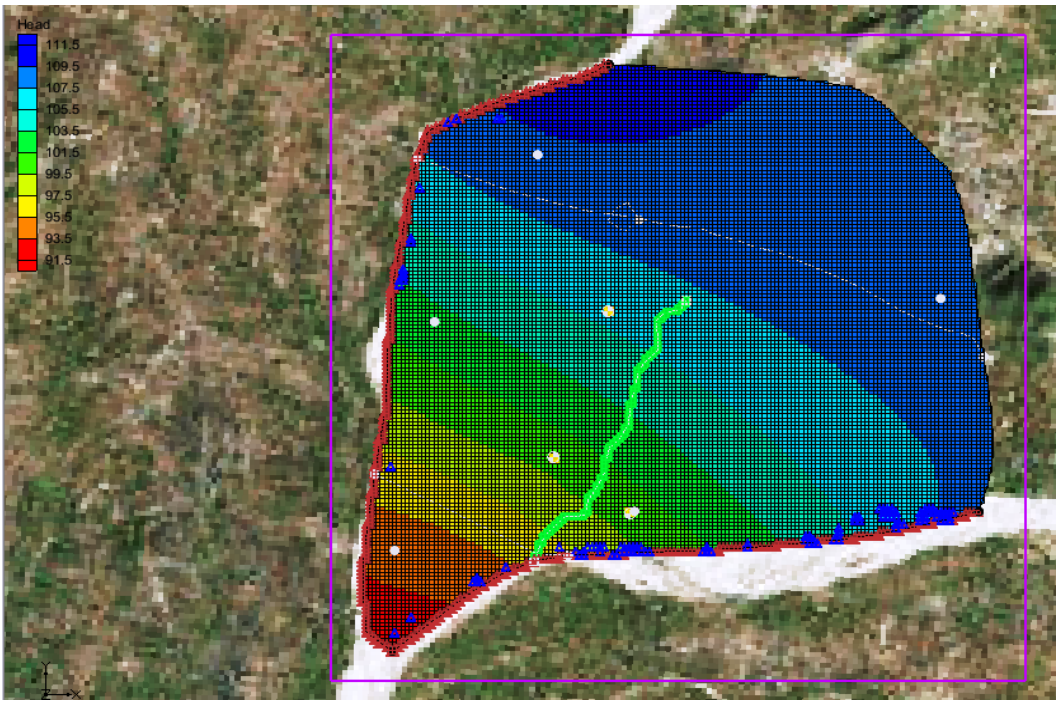


Fig.8: Flow Field obtained from MODFLOW execution

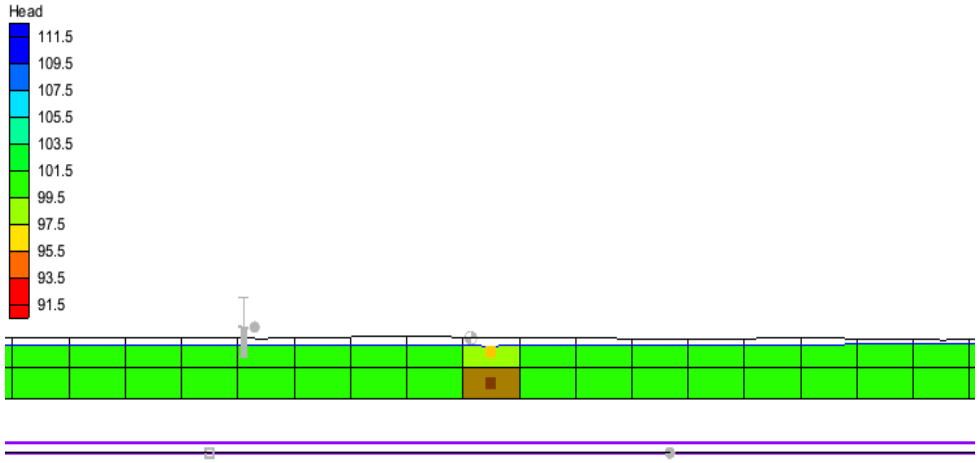


Fig.9: Water level near Row 110

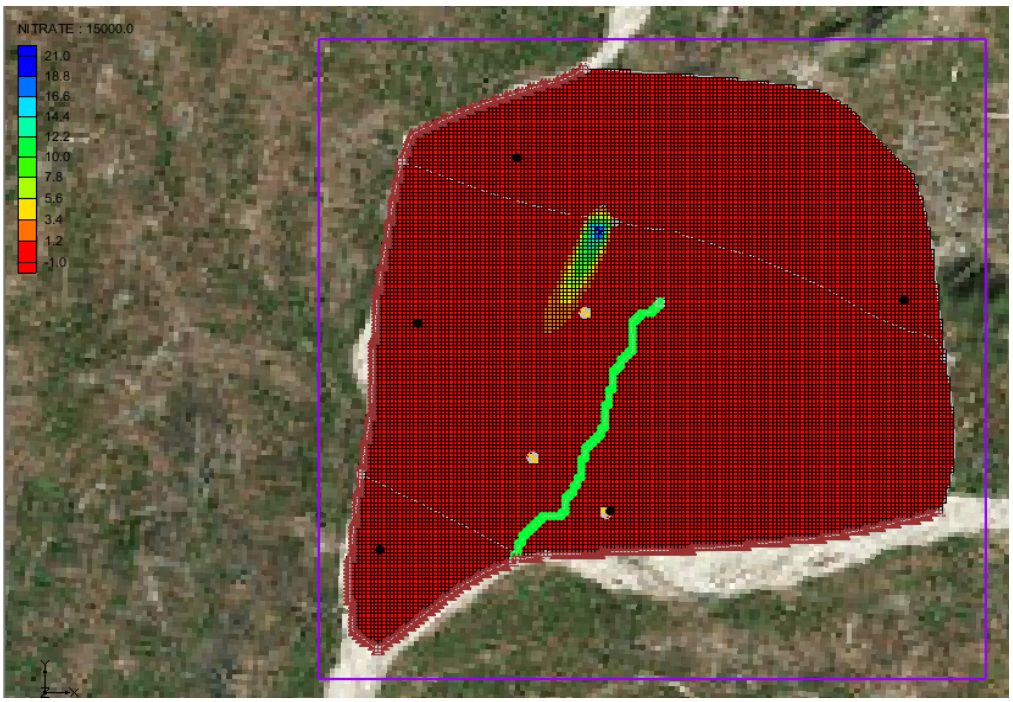


Fig.10: Contaminant transport after 20 years

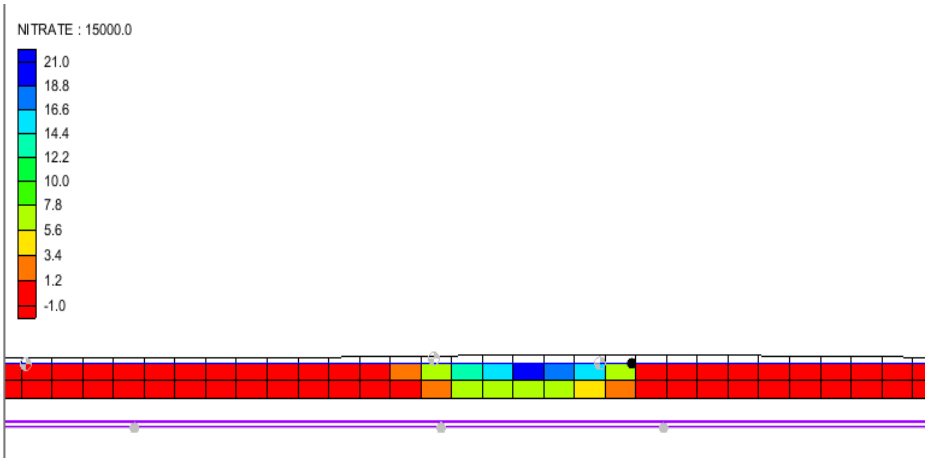


Fig.11: Transport of Nitrate (mg/l) near row 56

VI. CONCLUSIONS

A Conceptual model approach is more suitable over analytical approach to solve complex groundwater flow and contaminant transport phenomena and GMS has proven to be an effective tool. To evaluate the region on the bases of spread of contaminant, present research focused on hydro-geological data, climatic information, precipitation data, and stratigraphy knowledge to predict transport fate for 20 years.

The transport model shows the size of contaminant plume to be 360 meters in X direction and 600 meters in Y direction for layer 1. Aquifer layer 2 shows higher dispersion rates indicating higher concentrations resides in shallow zones but deeper zones are also getting contaminated with respect to time.

Results obtained from the application of conceptual model emerge to be genuine although lack of sufficient can question its validation. Thus, a monitoring well is needed to be set in the vicinity of contamination plume to observe gradual variations.

As a Future scope of this research, more descriptive conceptual model ensuring non monsoon recharge rates, a separate groundwater evapotranspiration package and a solid stratigraphy model should be applied to get accurate flow field. In transport model, chemical package should be involved indicating the changes from sorption and decay transport processes.

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