GROUNDWATER CONTAMINANT TRANSPORT MODELING USING MODFLOW and MT3DMS in TIRAP COAL FIELDS, TINSUKIA DISTRICT, ASSAM

***M. Tech 3rd semester Dissertation Phase 1 report** Submitted in Partial Fulfillment of the Requirements for the Degree of*

MASTER OF TECHNOLOGY

WATER RESOURCE ENGINERING

CIVIL ENGINEERING

2023-2025

Submitted by:

Name: Sonakshi Deori

MTech 3rd Semester

Roll no: PG/C/23/36

ASTU Roll no :230620061017

Guided by:

Dr. TriptiMoni Borah

Professor,

Civil Engineering Department,

Assam Engineering College

DEPARTMENT OF CIVIL ENGINEERING,

ASSAM ENGINEERING COLLEGE,

JALUKBARI, GUWAHATI - 781013

ASSAM ENGINEERING COLLEGE

JALUKBARI, GUWAHATI – 781013

CERTIFICATE OF SUPERVISOR

This is to certify that the work contained in the report entitled **"GROUNDWATER CONTAMINANT TRANSPORT MODELING USING MODFLOW and MT3DMS TIRAP COAL FIELDS, TINSUKIA DISTRICT"** submitted by-

SONAKSHI DEORI (PG/C/23/36)

A Student of M-Tech 3RD Semester to the Department of Civil Engineering, Assam Engineering College for the successful completion of the course **CEW202322 - DISSERTATION PHASE I report** as a partial fulfillment of the degree in **Master of Technology in Water Resource Engineering**, Civil Engineering, has been carried out under my guidance and supervision

Dr. Triptimoni Borah

Date:

Professor,
Department Of Civil Engineering
Assam Engineering College
Jalukbari,781013- India

ASSAM ENGINEERING COLLEGE

JALUKBARI, GUWAHATI – 781013

CERTIFICATE OF HEAD OF THE DEPARTMENT

This is to certify that the work contained in the report entitled **“GROUNDWATER CONTAMINANT TRANSPORT MODELING USING MODFLOW and MT3DMS INTIRAP COAL FIELDS, TINSUKIA DISTRICT, ASSAM”** submitted by-

SONAKSHI DEORI (PG/C/23/36)

A Student of M-Tech 3RD Semester to the Department of Civil Engineering, Assam Engineering College for the successful completion of the course **CEW202322- DISSERTAION PHASE I report as** a partial fulfillment of the degree in **Master of Technology in Water Resource Engineering**, Civil Engineering, has been carried out as per university protocols. The dissertation which is based on candidate’s own work has not been submitted to any other institution in any form

Dr. Jayanta Pathak

Date:

Professor & Head
Department Of Civil Engineering
Assam Engineering College
Jalukbari,781013- India

DECLARATION BY THE CANDIDATE

I, a student of the Department of Water Resource Engineering, Civil Engineering, Assam Engineering College, hereby declare that we have compiled this report on the topic titled **"GROUNDWATER CONTAMINANT TRANSPORT MODELING USING MODFLOW and MT3DMS" in LEDO, MARGHERITA"** in 3rd Semester as a part of my M. Tech curriculum.

I also declare that the same report or any substantial portion of this report has not been submitted anywhere else as part of any requirements for any degree/diploma etc.

Date:

NAME	**ROLL NO.**	**SIGNATURE**
Sonakshi Deori	230620061017	

ACKNOWLEDGEMENT

It gives me a great sense of pleasure to present the report on **“GROUNDWATER CONTAMINANT TRANSPORT MODELING USING MODFLOW and MT3DMS” in LEDO, MARGHERITA”** completed during my **M. Tech 3rd Semester**. I owe special debt of gratitude to **Dr Tripti Moni Borah**, Professor, CED of Assam Engineering College, Jalukbari, Guwahati for her constant support and guidance throughout the course of this work. Her, sincerity, thoroughness and perseverance have been a constant source of inspiration for us. It is only her cognizant efforts that my endeavors have seen the light of the day. I am highly indebted to her constant guidance and supervision as well as for providing full co- operation throughout the study and preparing the dissertation phase 1. Working under her has indeed been a great experience and inspiration for me.

I would also like to take this opportunity to thank the whole faculty of the department for their support and cooperation during the development of our project. Finally, I recognize the participation of my friends in the project's completion. Also, this project would not have been possible without the assistance of my seniors, whose benignant guidance helped me throughout the project.

It was a great source of motivation and helped me keep the momentum alive throughout this study.

TABLE OF CONTENTS

CONTENTS	Page No.
1. Introduction	10
2. Literature Review	12
2.1 Adeoye et al. (2018)	12
2.2 Sathe Sandip et al. (2018)	12
2.3 Kumar Anil et al. (2021)	12
2.4 Chowdhury Anupam et al. (2023)	12
2.5 Siharath et al. (2023)	13
3. Objectives of the Study	14
4. Methodology	15
4.1 Study Area	15
4.2 Software and Tools	16
4.3 Model Development	17
4.3.1 Conceptual Model	17
4.3.2 Data Used	18
4.4 Steps for Developing a Conceptual Model	22
4.4.1 Shapefiles of Study Area Inserted in GMS	22
4.4.2 Boundary Coverages for the Model	23
4.4.3 3D Grid and MODFLOW Simulation	24
4.4.4 DEM TIFF File Insertion	25
4.4.5 Interpolation to MODFLOW Layers	26
4.4.6 Mapping Coverages to MODFLOW	29
4.4.7 Running MODFLOW Simulation	30
4.4.8 Transition to Transient Model	32
4.4.9 Calibration of Transient Model	37
4.4.10 Introduction to MT3DMS	40
4.4.11 Aborted MT3DMS Runs	47

5. Results and Discussions. 51

5.1 Flow Budget Analysis 51

5.2 Transient Calibration Results 57

6. Conclusion 62

7. References 63

LIST OF TABLES

Particulars	Page no.
Table 4.4.1: Assumed Flow Rate of 10 Bore Wells	23
Table 4.4.2: Stress Periods Added to Transient Model	34
Table 4.4.3: Year vs Recharge Rate Data for Transient Calibration	37
Table 4.4.5: Bore Well Flow Rate Data with Start and End Date	38
Table 5.1 -5.7: Flow Budget Analysis Table of Transient Model Layers	50-63

LIST OF FIGURES

Particulars **Page no.**

Figure 4.1: Index Map of Study Area (Source: NEC) 15
Figure 4.2: Survey Map of Study Area (Source: NEC) 16
Figure 4.4.1: Shapefiles of Study Area inserted in GMS. 22
Figure 4.4.2: Boundary Coverages for the model 23
Figure 4.4.3: Creating 3D Grid and New MODFLOW Simulation 24
Figure 4.4.4: DEM TIFF File Insertion 25
Figure 4.4.5: Interpolate DEM File to MODFLOW Layers 26
Figure 4.4.6: Interpolation of Raster Data to MODFLOW Layers 27
Figure 4.4.7: Interpolated MODFLOW Layers 28
Figure 4.4.8: Map all the Applicable Coverages made to MODFLOW. 29
Figure 4.4.9: MODFLOW Run in Steady State 30
Figure 4.4.10: MODFLOW Simulated in Steady State 31
Figure 4.4.11: Model Changed to Transient Type 32
Figure 4.4.12: Assigned Layer Properties 35
Figure 4.4.13: Running State of Transient Model 36
Figure 4.4.14: The Pink Grid Represents Inactive Areas (Hilly Regions) 37
Figure 4.4.15: Transient Model after Calibration 38
Figure 4.4.16: First Approach Towards MT3DMS 40
Figure 4.4.17: Package Selection 41
Figure 4.4.18: Advection Package 42
Figure 4.4.19: Dispersion Package 43
Figure 4.4.20: Chemical Reaction Package 44
Figure 4.4.21: Assigning Properties in Tirap 45
Figure 4.4.22: New Polygon Created for Source Concentration 46
Figure 4.4.23: Aborted MT3DMS 47
Figure 4.4.24: Aborted in Steady State Considering Single Layer 49
Figure 4.4.25: Model Display after MT3DMS Abortion Figure 50

Particulars	Page no.
Figure 5.1: Layer 1 Flow Budget	51
Figure 5.2: Layer 2 Flow Budget	53
Figure 5.3: Layer 1 Flow Budget of Calibrated Mode	57
Figure 5.4: Layer 2 Flow Budget of Calibrated Mode	59

ABSTRACT

This study investigates groundwater contamination transport within the Tirap Open Cast Project (OCP) area in Tinsukia district, Assam, using MT3DMS modeling integrated into GMS. The Tirap OCP, located in the Makum Coalfields, is characterized by its complex geology, including alluvial aquifers with low hydraulic conductivity (0.01 m/day), making it highly susceptible to contaminant migration. The study focuses on understanding the transport and fate of any groundwater contaminant, to aid in developing remediation strategies.

A detailed conceptual hydrogeological model was developed based on subsurface data from exploratory drilling and geophysical surveys. The area features a multi-layer aquifer system with alternating aquifers and aquicludes, where the uppermost layer is an unconfined aquifer. Groundwater flow was simulated using MODFLOW, followed by contaminant transport modelling using MT3DMS. The model employed a 3D grid structure over a 222.08 km^2 effective area and incorporated boundary conditions, recharge rates, and hydraulic properties derived from field data.

The transport modelling considered advection, dispersion, and chemical reactions. Simulations revealed that recharge is the dominant inflow mechanism, while head-dependent boundaries contribute significantly to outflow. Results demonstrated the lateral and vertical spread of a Contaminant, with longitudinal dispersivity and molecular diffusion playing critical roles. The transient simulation provided insights into contaminant plume dynamics over a 100-year period, offering predictions on contaminant migration patterns.

Challenges included aborted MT3DMS runs due to excessive source/sink limits and system heterogeneity. Despite these issues, the study successfully calibrated the model, ensuring mass balance with negligible errors. Flow budgets across the aquifer layers indicated that recharge and storage significantly influence groundwater movement, with minimal discrepancies in inflow and outflow.

The findings highlight the utility of MT3DMS in predicting contaminant behaviour and identifying critical zones for groundwater protection. This study underscores the need for reactive transport modeling in future research to account for chemical degradation processes affecting contaminants like TCE (Tri Chloro Ethylene). Such approaches would enhance the accuracy of long-term predictions and provide a robust basis for designing targeted remediation strategies in vulnerable mining regions like the Tirap OCP.

1. INTRODUCTION

The study focuses on the Tirap Open Cast Project (OCP) in Tinsukia district, Assam. The region is characterized by alluvial aquifers with a hydraulic conductivity of 0.01 , making it susceptible to contaminant transport.

Tirap Colliery is one of the three operating opencast mines of NEC and has been in existence since 1983. It is located in the Makum Coalfields of Assam. The Coalfields extend along the Northern front of the Naga–Patkai hill range. The coal seams have drained into folds (Anticline) plunging E-N.E. with the folds running more or less N.E – S.W. At present, workings are concentrated along the south limb of the anticlinal coal bed. Tirap OCP is located in the eastern extremity over the anticline in the northern limb of Makum coalfield. In the mine three main seams are being worked viz. 8Ftseam, 20Ft seam and 60Ft seam. Tirap OCP project lies in the south-west portion of Tirap underground Block which is in continuation of existing Tirap OCP in the dip side towards south and south- western side from the present working face and stretches up to Ledopani nala. The formations within the southern part of the study area belong to the Barail group of Oligocene age comprising Tikak Parbat and Baragolai formations. Out of the above, Tikak Parbat is the most important formation of the coalfield, since it contains the coal seams of the area. The rock types in Tikak Parbat formation are predominantly fine to medium grained sandstone with beds of sandy shales, mudstone, carbonaceous shale and coal seams. The northern part of the study area is covered with alluvial deposits of recent age. The dip and strike of the beds show variation commensurate with the pattern of folding with varying strike of N-S to E-W. The eastern and western limbs dip 20º southerly to 23º easterly. The dip is shallow in the axial region and varies from 8º to 15º easterly. In the northern limb the dip is steep with about 33º northerly. The dip is uniformly steep with 25º easterly in the southern part of the block. Margherita thrust lies north of Tirap opencast project area. Four faults have been identified in the Tirap OCP mine area. Three coal seams attaining workable thickness have developed in the project area namely 8’ seam, 20’ seam and 60’ seam. The maximum mine depth has been projected as 330 m.(CMPDIL).

Key Words: Contaminant transport modeling, Groundwater simulation, Groundwater contamination, Groundwater modeling, MODFLOW, MT3DMS.

2. LITERATURE REVIEW

2.1 Adeoye et.al (2018) used Visual MODFLOW to study the loading, dynamics fate and transport of some heavy metals in Minna shallow aquifer while MT3DMS was used to predict the concentration of the heavy metals in one, three- and five-years' time. Conceptual model approach was employed for the simulation with the model domain discretized into 50cells each in *x* and *y* directions. Results showed that the whole aquifer was strongly contaminated with arsenic, copper and Zinc. This was presented as colour shading by visual MODFLOW. Initial concentrations of arsenic copper and zinc were 0.74mg/L, 8.43mg/L and 11.63mg/l respectively as against 0.01mg/l, 2.00mg/L and 5.00 mg/L recommended as maximum allowable contamination (MAC) for drinking water by WHO. MT3DMS predicted a progressive reduction in heavy metals concentration. For instance, a reduction in value to 0.60 mg/L, 7.51 mg/L and 4.20 mg/l were predicted for arsenic, zinc and copper respectively over five-years period. The study also revealed that the polluted shallow aquifer in Minna can be cleaned up of these heavy metals after some years.

.

2.2 Sathe Sandip et.al. (2018) studied on understanding arsenic contamination in the groundwater of Bongaigaon and Darrang districts in the Brahmaputra floodplain, India. It uses 3D groundwater flow and contaminant transport models to predict contamination patterns and evaluate mitigation strategies. Arsenic contaminated shallow aquifers evaluation, mitigation, and management strategies are the challenging task to all the hydrologist and to provide a safe drinking water demand in the Holocene age, alluvial aquifers. To manage and mitigate such problems, they used numerical groundwater modeling software (GMS 10.2), for the development of 3D transient state predictive (groundwater flow and contaminant transport) conceptual model for two topographically different arsenic contaminated regions. The models were built by using the measured hydro-geological data, empirical values, and equations. Groundwater flow calibration, sensitivity analyses, and validation were performed for each soil parameters, varying boundary conditions and for alternate meteorological scenarios.

2.3 Kumar Anil et.al (2021) presented the results and inferences drawn from studies on pollutant migration from chemical and pharmaceutical industries established around the Choutuppal Industrial Area near Hyderabad. Partially effluents whether treated or untreated were discharged from these industries directly onto the surface, into streams, polluting surface and groundwaters. In order to estimate the extent of pollution, an experimental study integrated with the application of MT3DMS was carried out. As a part of experimental investigation, the close monitoring of groundwater level and water quality was carried out. The preparation of Mass transport models was made using visual MODFLOW software with a discussion on the spatial (vertical and horizontal) and temporal expansion of plume of contamination of groundwater at different subsurface formations in the study area.

2.4 Chowdhury Anupam et.al (2023) studied *"Groundwater contaminant transport modeling using MODFLOW and MT3DMS: A case study in Rajshahi City"*, that focuses on assessing groundwater contamination in Rajshahi, Bangladesh, due to pollutants from an unlined landfill. It uses MODFLOW for groundwater flow modeling and MT3DMS for contaminant transport simulation. The study results showed that the migration distance of the contaminants increases over time and follows a logarithmic trend. Among the contaminants, the model-predicted results show that the concentration of Cr and Pb in the groundwater varies more than 90% from their standards over the period of 50 years, which suggests that these two pollutants are the prime contaminants polluting groundwater in the coming future. This model can be used as an effective decision-making tool for the monitoring of groundwater contaminant transport for a specific location

2.5 Siharath et.al. (2023) studied about the employing of the M3TDMS package as excellent tools to establish the 3D conceptual model of contaminant transport modeling, simulate and predict the multispecies of Lead and zinc substances which transport in the groundwater, there are 15 boreholes that were observed and monitored, the results of the contaminant transport modeling was found the Lead(Pb) contaminant transport with initial concentrations of 3.96 mg/l at borehole MB48 as point source, the concentration reduced to 0.1 mg/l, after 3,650 days simulation. The initial zinc (Zn) concentration of 0.886 mg/l at borehole CV04 decreases to 0.023 mg/l after 3,650 days simulation.

3. OBJECTIVES OF THE STUDY

- The main objective of the present study is to investigate groundwater quality in Tirap Coal fields in the district of Tinsukia.

- The groundwater model **MODFLOW** will be used to simulate the direction, velocity and distribution of groundwater flow.

- To solve Ground Water Flow Equation using GMS (MODFLOW) package i.e. FINITE DIFFERENCE METHOD.

- To evaluate the flow of groundwater contaminant and its extent due to continuous pumping.

4. METHODOLOGY

4.1 Study Area

The study focuses on the Tirap Open Cast Project (OCP) in Tinsukia district, Assam. The region is characterized by alluvial aquifers with a hydraulic conductivity of 0.01, making it susceptible to contaminant transport.

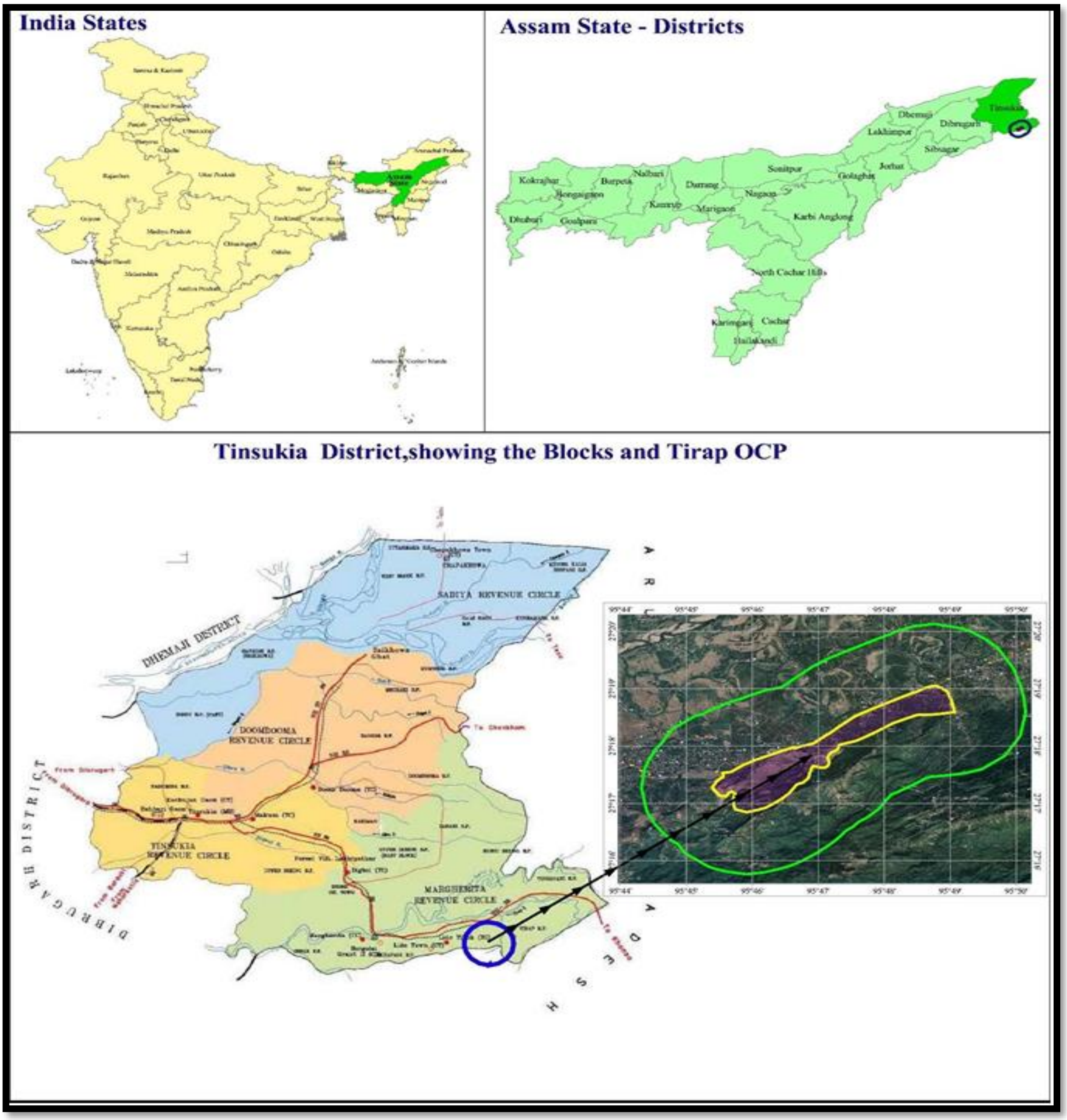


Fig 4.1: INDEX MAP OF STUDY AREA (source: NEC)

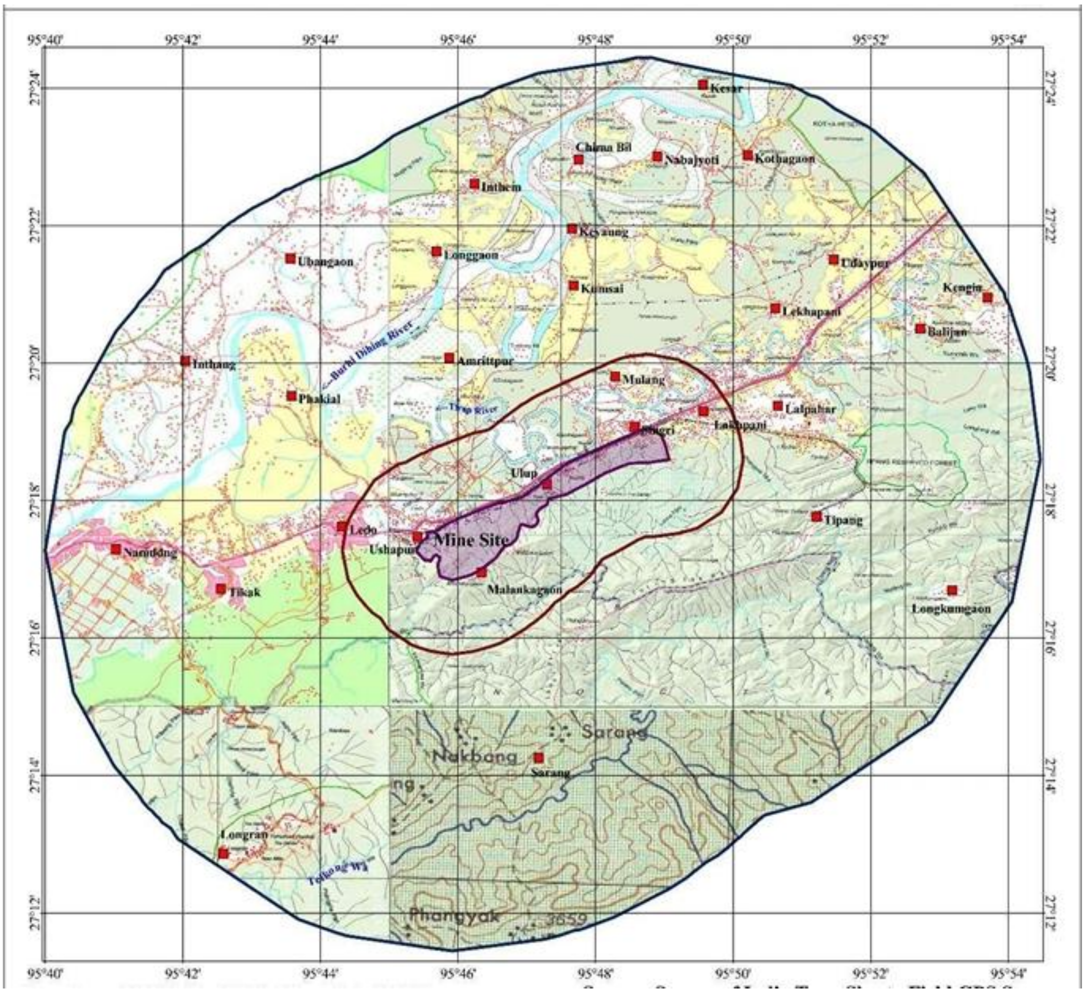


Fig 4.2: SURVEY MAP OF STUDY AREA (source: NEC)

The mine is located in the Makum Coalfields of Tinsukia district of Assam state, India. The mine is well connected by road and railways. The nearest railway station is Ledo, which is located at a distance of nearly 3 km on the Dibrugarh-Tinsukia, Lekhapani section of Northeast Frontier Railway zone. The NH 38 runs along the Northern part of this Colliery. The nearest town is Ledo and is about 3 km to the West of Margherita Township, which is the area H.Q of NEC situated at a distance of 10 km from the mine. The nearest domestic airport Mohanbari (Dibrugarh) is at a distance of 93 km from the mine. The mining block lies about 7 km southeast of Margherita town, the headquarters of the NEC. The study area (covering a 10 km radius) lies between North Latitude, 27° 11' 45" and 27°24'05" and East Longitude of 95°40'00" and 95°54'15". The Mine falls in 83M/15. The total aerial extent of the study area covering a 10 km radius from the mine boundary is 425.68 km^2.

4.2 Software and Tools

MT3DMS, integrated within GMS, was selected for this study due to its ability to model advection, dispersion, and chemical reactions of contaminants. The key features used include:

- **Advection:** Simulating the movement of contaminant due to groundwater flow.
- **Dispersion:** Accounting for the spreading of the contaminant.
- **Diffusion:** Incorporating molecular diffusion effects.

4.2.1 EQUATIONS INVOLVED IN CONTAMINANT TRANSPORT

a) DIFFUSION ADVECTION EQUATION

$$\partial C/\partial t + V\cdot\nabla C = \nabla\cdot(Dh\cdot\nabla C) - R$$

- C is the variable of interest (species concentration for mass transfer, temperature for heat transfer),
- D is the diffusivity (also called diffusion coefficient), such as mass diffusivity for particle motion or thermal diffusivity for heat transport,
- v is the velocity field that the quantity is moving with. It is a function of time and space.
- R describes sources or sinks of the quantity c, i.e. the creation or destruction of the quantity.
- ∇ represents gradient and ∇ · represents divergence. In this equation, ∇c represents concentration gradient.

b) The flow of groundwater through porous media is governed by **Darcy's Law** and the principle of **mass conservation**, resulting in the **groundwater flow equation:**

$$Ss.\ \partial h/\partial t = =\nabla\cdot(K\nabla h)+W$$

- h: Hydraulic head (L)
- t: Time (T)
- Ss: Specific storage L^ {-1}
- K: Hydraulic conductivity tensor (L/T)
- ∇h: Hydraulic gradient (L/L)
- W: Source/sink term (L/T) (e.g., recharge or pumping)

c)General governing equation for steady-state, heterogeneous, anisotropic conditions, without a source/sink term

$$\frac{\partial}{\partial \varkappa}\left(k_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial h}{\partial z}\right)=0$$

d)General governing equation for steady-state, heterogeneous, anisotropic conditions, with a source/sink term

$$\frac{\partial}{\partial \varkappa}\left(k_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial h}{\partial z}\right) = -R *$$

e) General governing equation for transient, heterogeneous, and anisotropic conditions

$$\frac{\partial}{\partial \varkappa}\left(k_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial h}{\partial z}\right) = Ss \frac{\partial h}{\partial t} - R *$$

Where S_s refers to specific storage.

4.3 Model Development

4.3.1 Conceptual Model

The entire study area forms part of the Carbonaceous sandy shale, Sandstone & Coal seams and Ferruginous sandstone. As per the subsurface exploratory drilling carried out by the CMPDIL and CGWB, there exist a multi-layer aquifer system. After the detailed study of the subsurface borehole data, three aquifer systems of the six-layer concept (i.e., 3 aquifers and 3 aquicludes) have been identified for the purpose of ground water modeling in the region, and appropriate layers and aquifer parameters are assigned for understanding the prevailing flow regime. The model area covers around 425.68 km^2 and the effective area considered for modelling is 222.08 km^2 after excluding the hill areas which acts as runoff zone. The details of the model structure are explained in the following sections. The details about the conceptual model are given in Table 4.3.1.

Table 4.3.1 Details about the conceptual model

Parameter	Value	
Grid	Grid Size in m	200 X 200 m
	No. of Column	120
	No. of Row	121
	No. of Active Grid	5554
	No. of Inactive Grid	5088
Top of aquifer (m) range of elevation	Surface Elevation: 97.56 – 1114.22 m	
Bottom of aquifer (m) range of elevation	Bottom Layer: -50.47 to 1012.93 m	
Initial Piezometric Heads (m AMSL)	Layer 1	139.50 – 327.78 m
	Layer 2	-
	Layer 3	-
Aquifer Type	Layer 1	Phreatic aquifer
	Layer 2	Aquiclude-1
	Layer 3	Aquifer with less potentiality (Semi-confined)
	Layer 4	Aquiclude-2
	Layer 5	Aquifer with less potentiality (Semi-confined)
	Layer 6	Aquiclude-3

	Drain Boundary Condition River Boundary Condition Recharge Boundary Condition	
Boundary Conditions Used	Well Boundary Condition	
	Layer 1	1
	Layer 2	0.1
	Layer 3	0.5
K (m/ Day)	Layer 4	0.1
	Layer 5	0.5
	Layer 6	0.1
Specific yield (%)	Layer 1	2%
Storage Parameters	Layer 1	0.02
	Layer 2	0.013
Recharge applied	200-220 mm/year *(Based on the CGWB Ground Water Estimation Committee-2015 Norms)*	

Table 4.3.1 Details about the conceptual model contd.

4.3.1.2 Data Used while developing a conceptual model.

a) Boundary Shapefiles of the study area i.e. Tirap mine collinery collected from Coal India Limited

b) Well Shapefiles of the study area collected from Coal India Limited

c) Flow rate and Pumping rate of wells collected from Coal India Limited

d) Hydraulic parameters and boundary conditions collected from Coal India Limited

The ground elevation has been generated using SRTM DEM (30 m) for the model area. From the surface elevation, the layer thickness is generated based on the interpolation of the lithology data, well inventory data, and geophysical survey interpreted results. The reduced level surface has been generated and the same is used as input layers for the model. The hydraulic conductivity values are distributed for these six layers/formations based on APT results. The hydraulic conductivity (kx=ky) for each layer ranges from 1.0 m/day to 0.1 m/day. The higher conductivity is given for the top layer and then the coal seam owning a minimum of 0.1 m/day (Table 4). Vertical hydraulic conductivity (kz) has been taken as 10% of the horizontal hydraulic conductivity. The Specific yield of 2% is assigned to the topmost layer/ unconfined aquifer in the model are :

4.3.1.2 Mathematical Model

M3TDMS package consists of contaminant transport modeling, which obviously applied the 2 or 3-dimensional of advanced mathematical equation to elaborate from physical to mathematical model (Jacob Bear , Alexander H.-D. Cheng, 2010) , the PDE will be employed in the movement of advection, diffusion in the groundwater contaminant transport modelling (Gerald W. Recktenwald, 2011).

1. Initial Condition

Most of the models were employed numerical method to simulate the groundwater modelling, Therefore, prior to dealing with and finding the precise results, initial condition is required to identify to support the groundwater modeling, the governing equation shows as below:

$$C(x, y, z, t) = c_0(x, y, z) \quad \text{on } \Omega, t \geq 0$$ Where C(x,y,z,t) are known concentrations

2. Boundary Condition

Boundary condition also plays an important role for contaminant transport modeling to model the chemical substances in groundwater modelling. Additionally, there are three types of boundary conditions to apply in contaminant transport modeling (MT3DMS) (Siharath phoummixay and Guillermo III Quesada Tabios,2020, Philip B., et al., 1994) such as:

- **Dirichlet**: the concentration is specified along the boundary for the entire duration of the simulation

$$C\,(x, y, z,\ t) = c\,(x, y, z,\ t)\ , \qquad \text{on } \Gamma_1,\ t \geq 0 \quad \text{(b)}$$

Where: the specified concentration boundary,

Specified concentration along. The specified concentration may be set to vary with time.

- **Neumann**: the concentration gradient is specified across the boundary.

$$\theta D_{iJ}\left(\frac{\partial C}{\partial x_J}\right) = f_i(x, y, z, t) \qquad \text{on } \Gamma_2,\ t \geq 0 \quad \text{(c)}$$

Where: Known function representing the dispersive flux normal to the

boundary, a special case is a no dispersive mass flux boundary where

$f_i(x,y,z,t) = 0$

- **Cauchy**: The Cauchy boundary condition, both concentration value and concentration gradient are specified.

$$\theta D_{iJ}\left(\frac{\partial C}{\partial x_J}\right) - q_i C = g_i(x, y, z, t) \qquad \text{on } \Gamma_3,\ t \geq 0$$

4.4. STEPS FOR DEVELOPING A CONCEPTUAL MODEL and MT3DMS

STEP 1: Open GMS and project the shapefiles

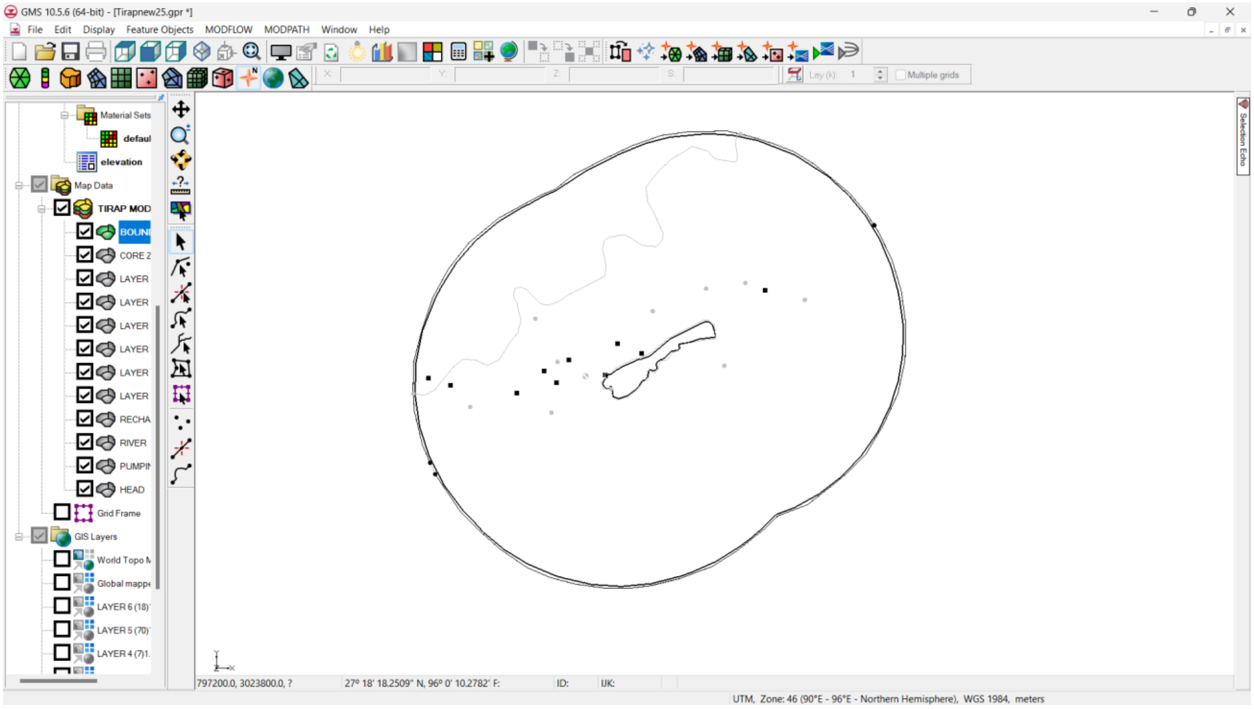


Fig 4.4.1 Shapefiles of study area inserted in GMS

Firstly, the collected shapefiles were imported (provided by CMPDI) in GMS

After that projection was made for this area as falls under WGS 1984 UTM ZONE 46N

World Topo Map was added so that Arcs and polygons could be drawn to make coverages. In the later part of the methodology River coverage was made through arcs.

STEP 2: Making Boundary coverages for all the layers including river, wells and recharge and inserted the required values.

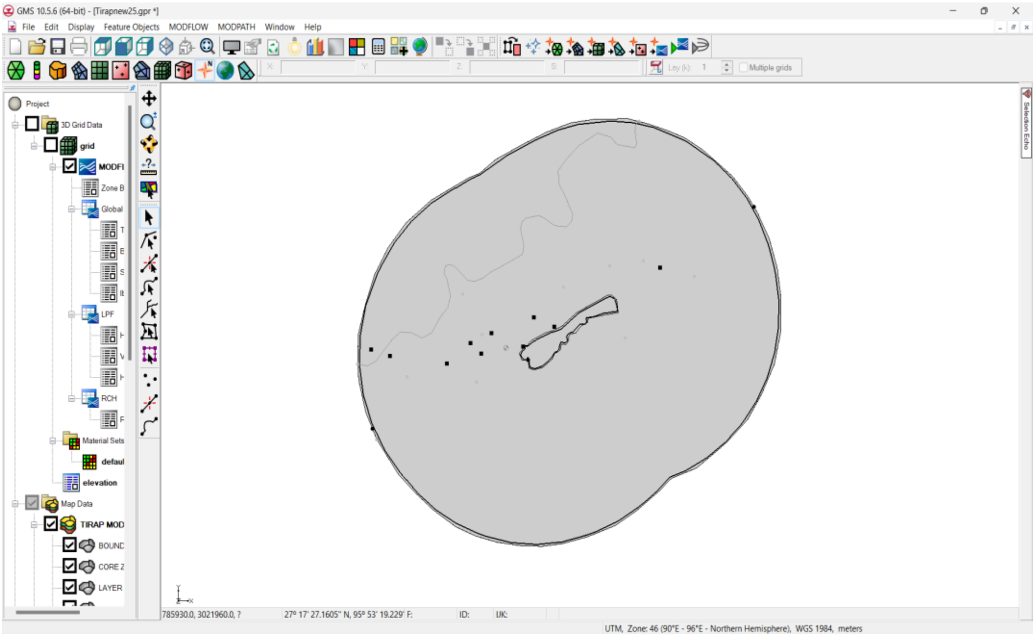


Fig 4.4.2: Boundary Coverages for the model

Boundary conditions are defined along the edges of the simulation domain including the top and the bottom. Their main function is to separate the model region from the rest of the world and are required for the solution of the ground water flow equation.

The river flow in the study area has been assigned with **River boundary condition** as the river flows in the pediment is not that prominent. There is no major reservoir in the study area of a 10 km radius; hence no constant head boundary has been assigned and considered a General Head Boundary with a conductance of 0.2 (m^2/day) (m).

Recharge boundary condition is defined in the top layer (As per GEC-2015 Norms) of 0.000624.

Also **10 Bore Well boundary condition** is defined with different flow rates are assumed .

Table 4.4.1: Assumed Flow rate of 10 Bore Wells

BORE WELLS	FLOW RATE (m^3/day)
BW 1	-500
BW 2	-850
BW 3	-700
BW 4	-950
BW 5	-500
BW 6	-700
BW 7	-700
BW 8	-678
BW 9	-600
BW10	-500

Flow rates of Bore Wells were assumed as it was unavailable

A **bore well** is a deep, narrow well drilled into the ground to access groundwater. It is typically created using specialized drilling equipment and is commonly used for agricultural, industrial, and domestic water needs in areas where surface water sources are insufficient. Bore wells can penetrate to depths ranging from a few tens to hundreds of meters, depending on the geological conditions and the water table.

STEP 3: Create 3D Grid and new Modflow simulation.

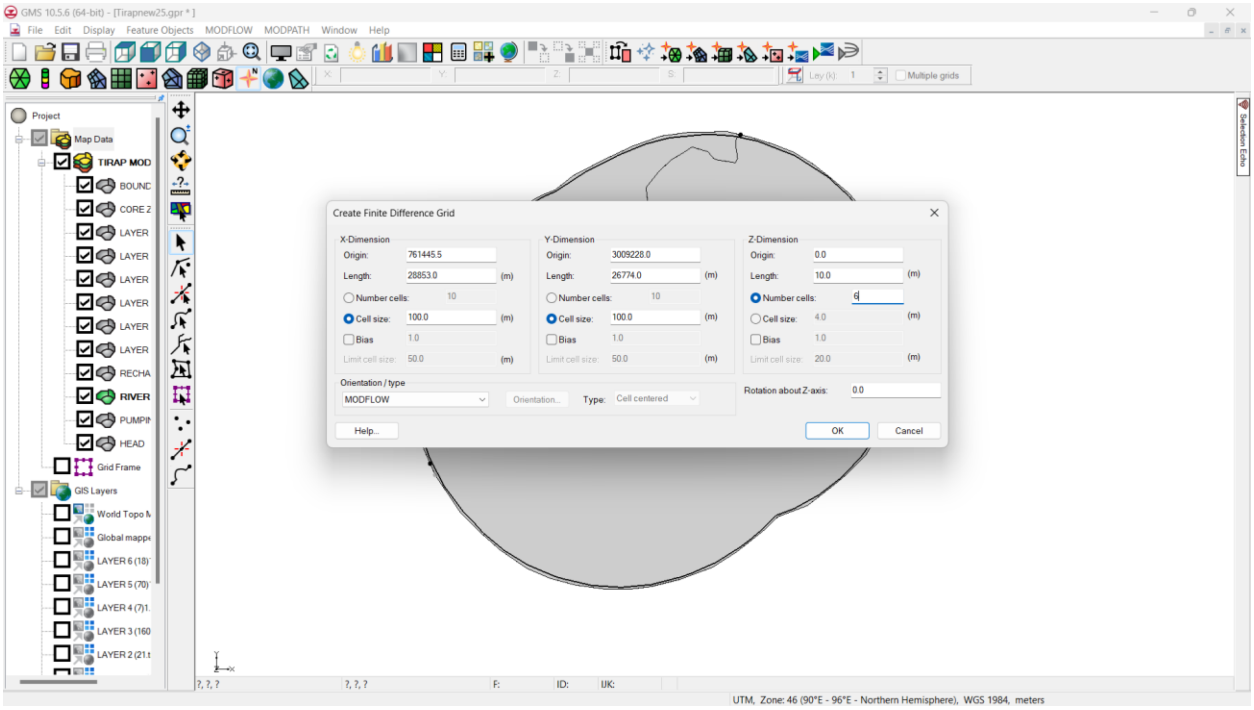


Fig 4.4.3 Creating 3D grid and new modflow simulation

The model grid of 100 X 100 m has been generated with 120 columns and 121 rows evenly distributed throughout the model domain. The entire model domain is represented by 10642 cells, out of which approximately 5554 cells are active cells, and 5088 cells are inactive

STEP 4: INSERTING THE DEM TIFF FILE OF THE STUDY AREA

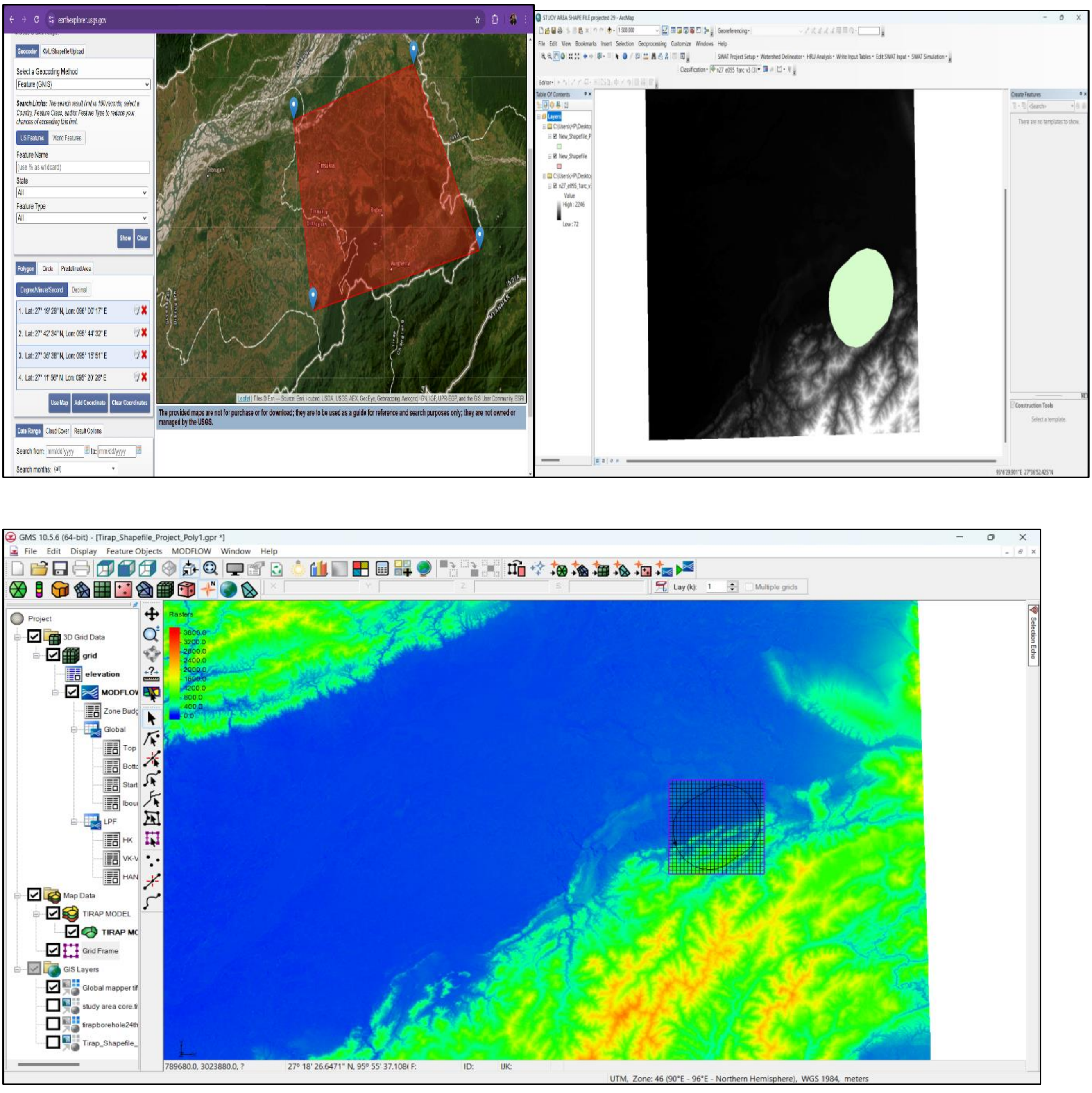


Fig 4.4.4: DEM TIFF file insertion

The DEM file was downloaded from USGS EARTH EXPLORER in Tiff format which was later set for projection in ARC-GIS and was exported to GMS Profile.

STEP 5: INTEPOLATION TO MODFLOW LAYERS

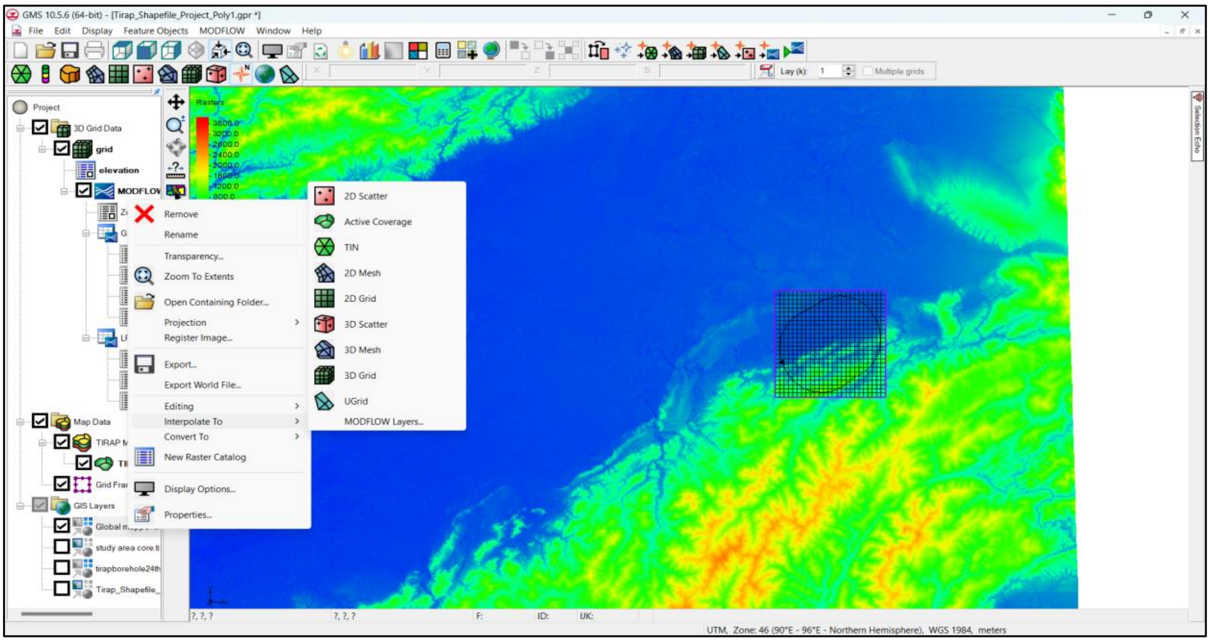


Fig 4.4.5 Interpolate DEM FILE TO MODFLOW Layer

Interpolation of DEM file is necessary as MODFLOW requires the top and bottom elevations of each model layer to define the geometry of the groundwater system. DEMs provide surface elevation data, which is often used to set the top elevation of the uppermost layer or to infer subsurface layer boundaries.

DEM interpolation ensures that the layer elevations reflect spatial variations in topography and geology, which are critical for accurate simulation of groundwater flow

STEP 6: INTERPOLATION OF RASTER DATA TO MODFLOW LAYERS

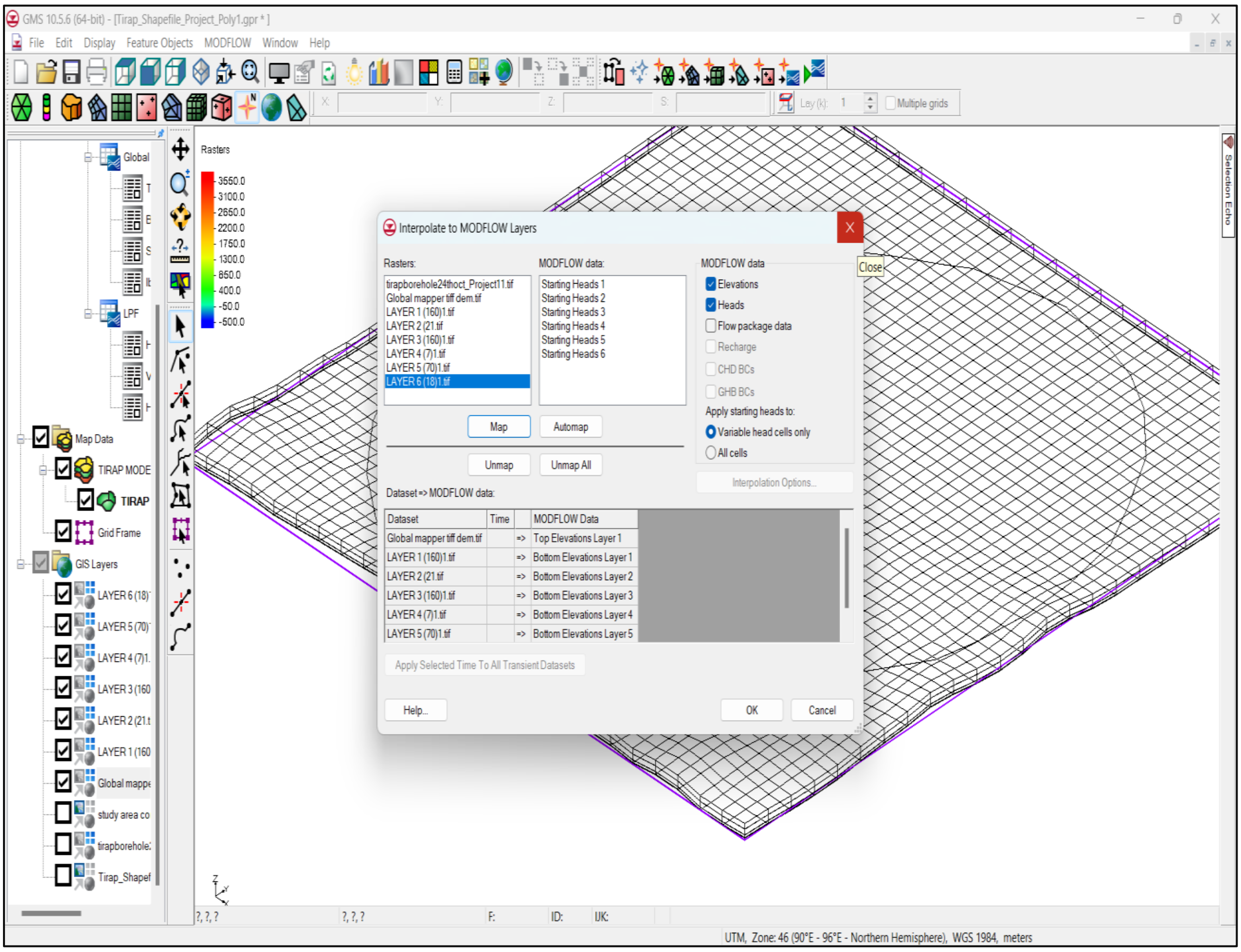


Fig 4.4.6: Interpolation of Raster to Modflow by Layers

DEM layer interpolation in GMS involves mapping elevation data from a Digital Elevation Model (DEM) onto the grid of a MODFLOW model to define the top and bottom elevations of model layers. The process starts by importing the DEM into GMS and ensuring it aligns spatially with the MODFLOW grid. The DEM is then interpolated to the grid using methods such as inverse distance weighting (IDW), kriging, or nearest neighbor to assign elevations to the model's top surface and, optionally, to define the bottom surfaces of subsequent layers. After interpolation, results are visualized using cross-sections or 3D views, and any inconsistencies are manually corrected or refined through re-interpolation. The final interpolated layers serve as the foundation for the MODFLOW model, representing the physical geometry of the modeled system

INTERPOLATED LAYERS

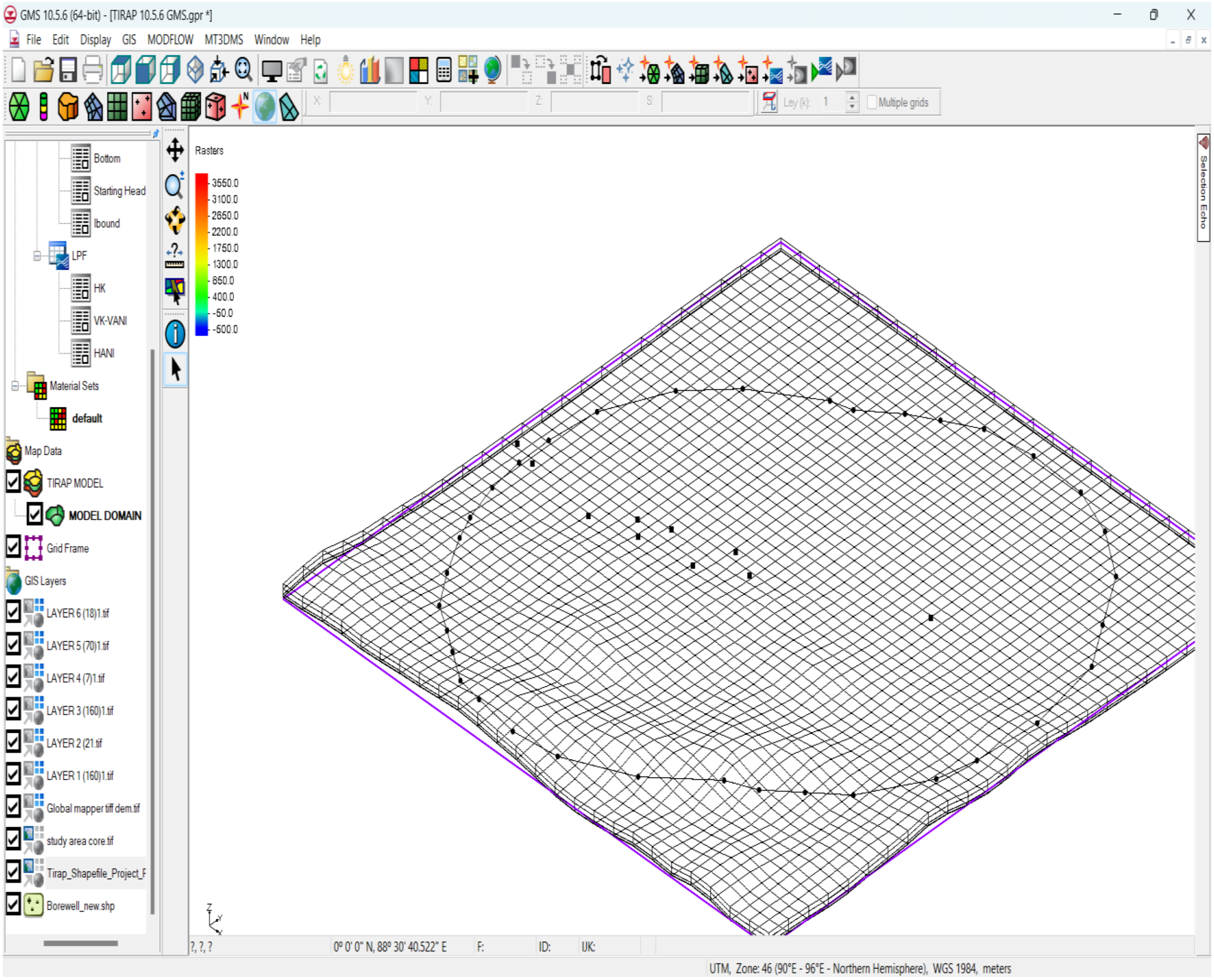


Fig 4.4.7: Interpolated Modflow layers

Fig 4.6 depicts how the layers of the aquifer got interpolated with the DEM and formed elevations near the hilly area.

STEP 7: Map all the applicable coverages made to Modflow

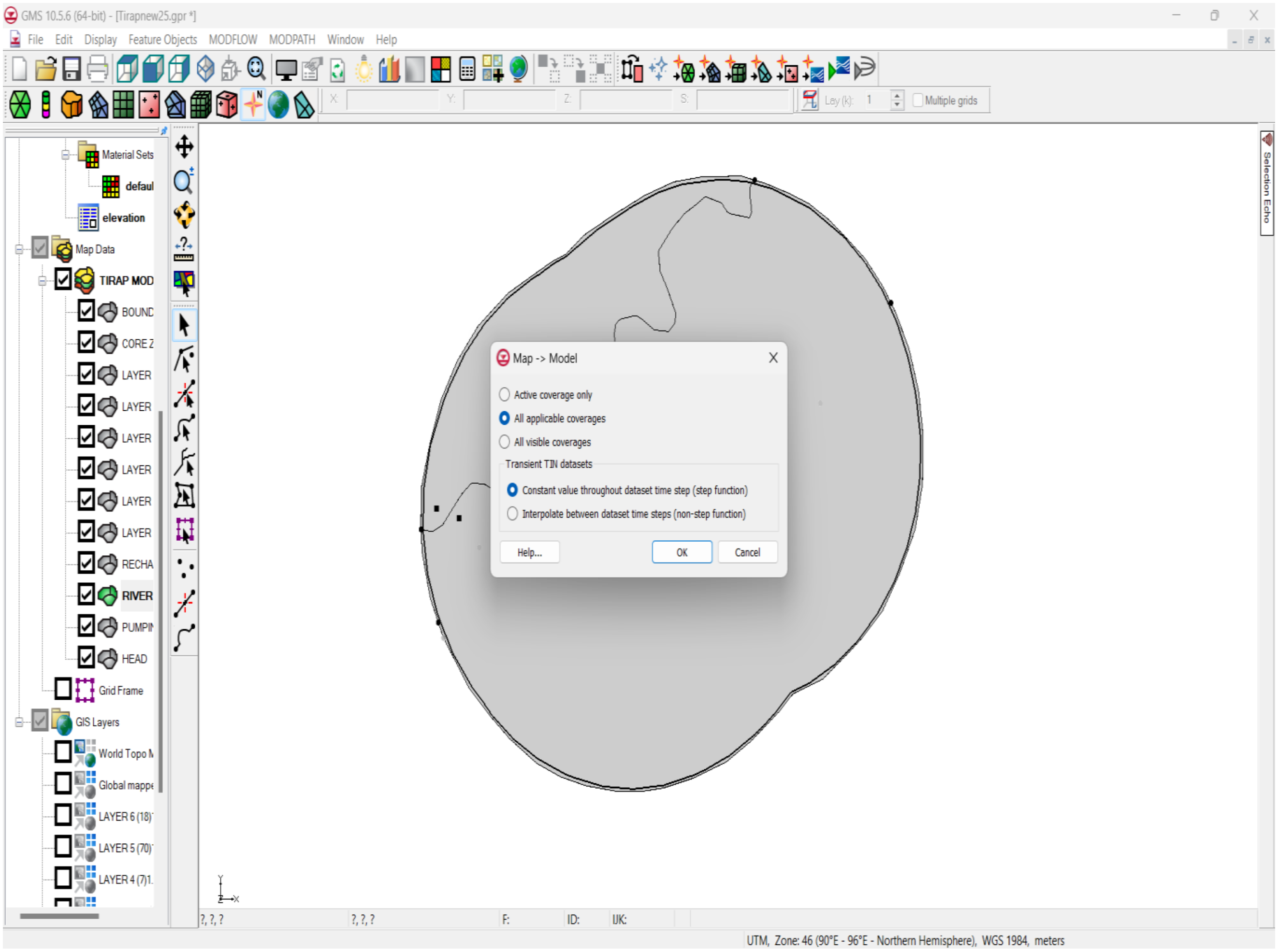


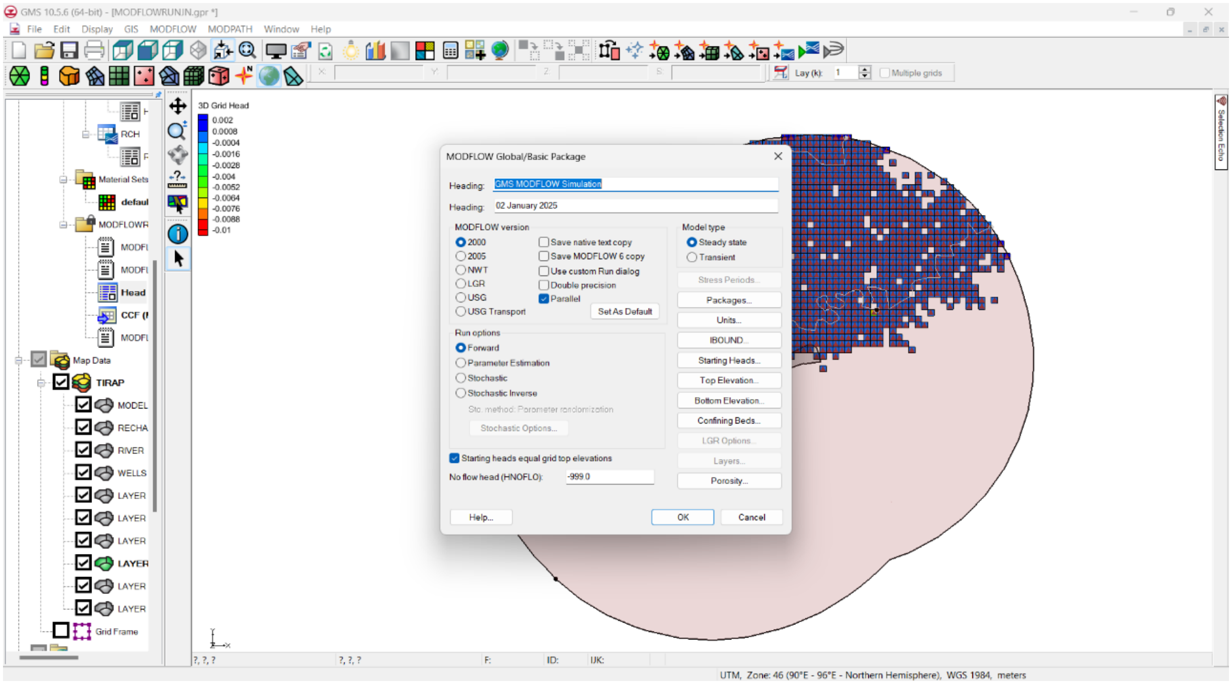
Fig 4.4.8: Map all the applicable coverages made to Modflow.

Mapping of coverages is necessary because coverages serve as a foundational component for defining and managing spatial and attribute data for various aspects of a groundwater model.

• Coverages allowed us to define the spatial boundaries of the model domain, such as the extent of the study area, subregions, or aquifers.

• Here in fig4.7 it enabled the representation of features like rivers, wells, recharge zones, which are crucial inputs for groundwater flow models.

STEP 8: RUN MODFLOW IN STEADY STATE



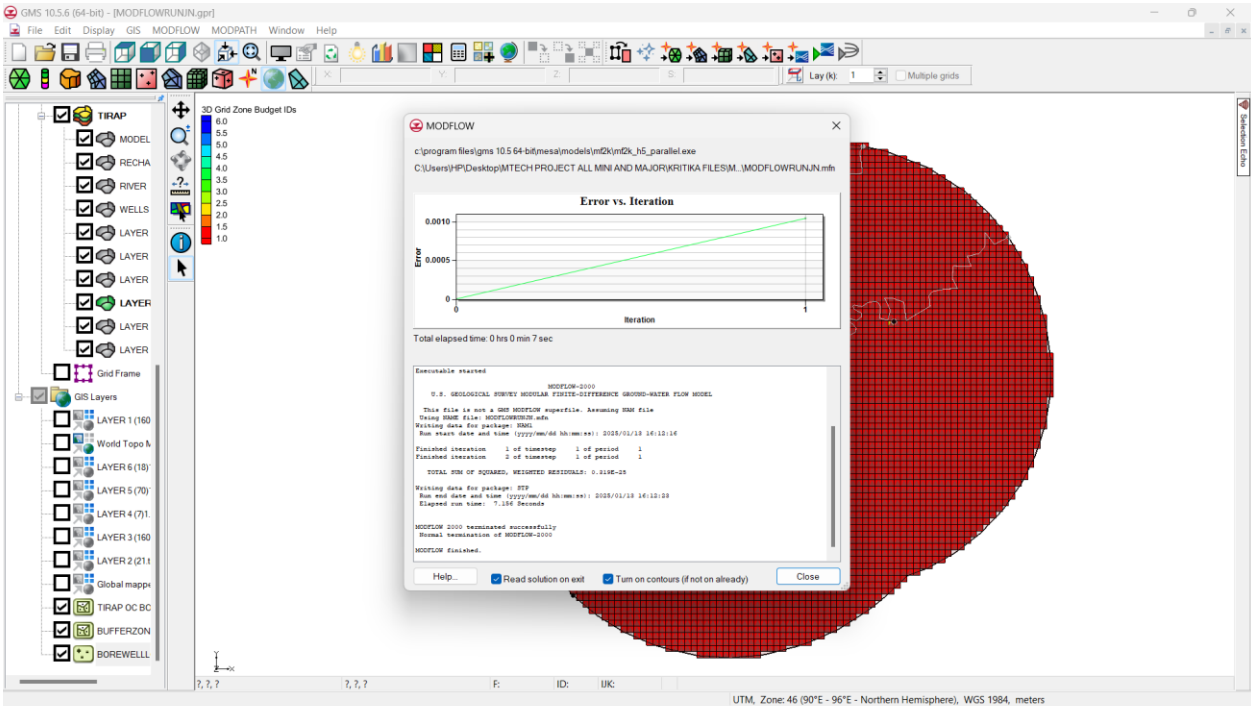


Fig 4.4.9: Modflow run in Steady State

STEP 9: MODFLOW SIMULATED IN STEADY STATE

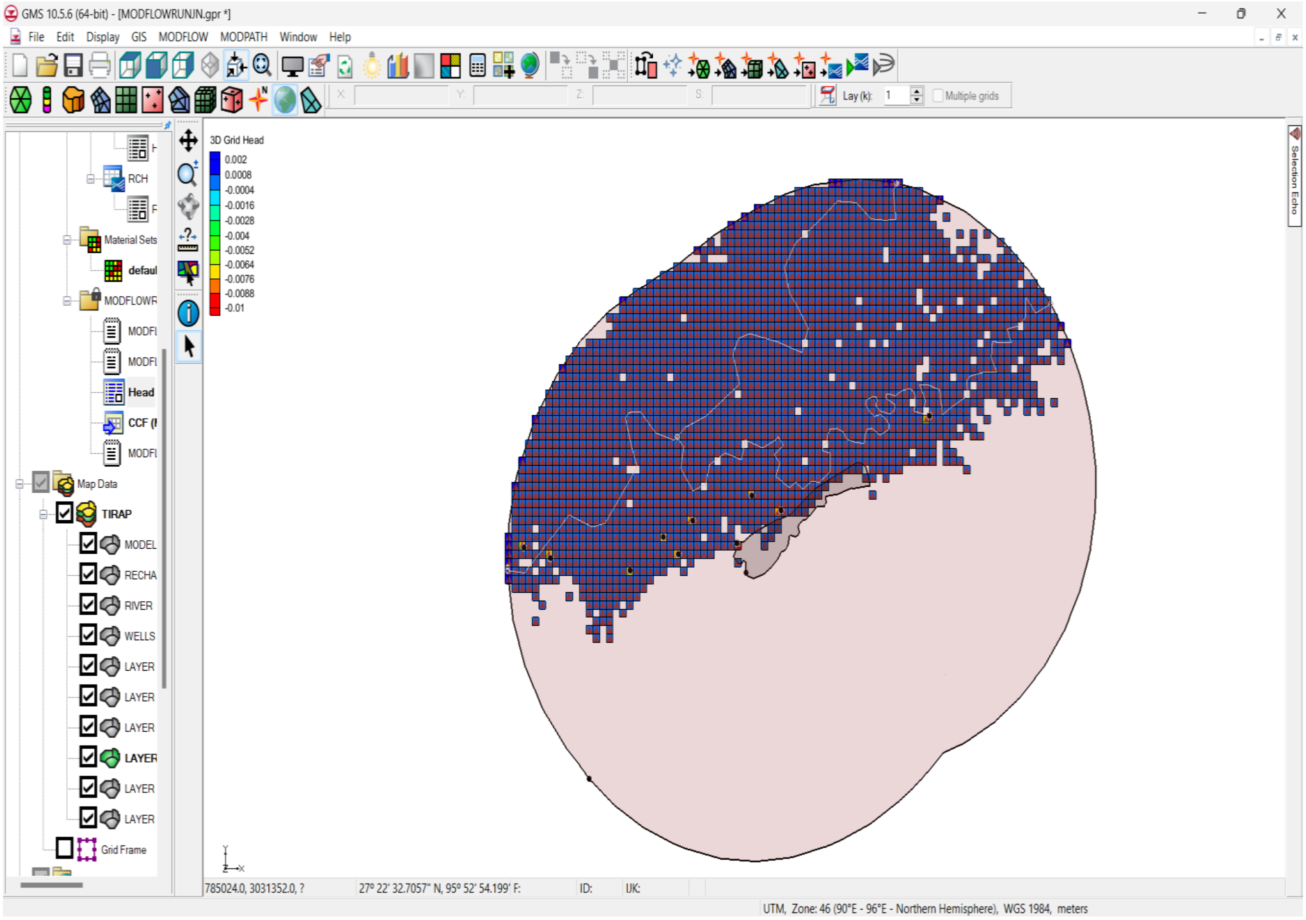


Fig 4.4.10 - Modflow Simulated in Steady State

The model was simulated in a steady-state condition, but the Hydrogeological framework of the model area is heterogeneous in nature, where the head change is never constant (i.e., the inflows and outflows are not equal). Therefore, transient simulation was attempted, and accordingly, the predictions are made in the transient run.

STEP 10: CONVERT MODEL TO TRANSIENT BY ADDING STRESS PERIODS

To change the model from Steady to Transient State , in the Modflow Global package options we change the model type to Transient and add some stress periods

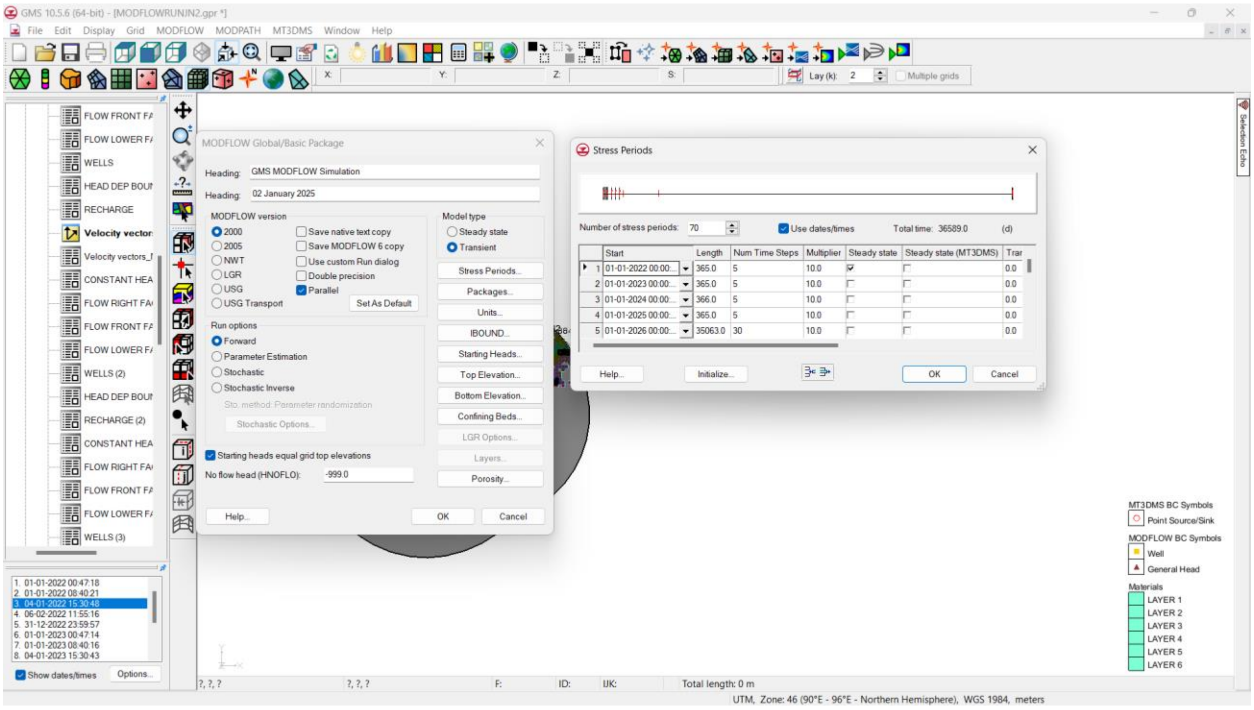


Fig 4.4.11: Model Changed to Transient type

A **stress period** is a discrete time interval in a transient simulation during which the external stresses on the groundwater system, such as pumping rates, recharge, or boundary conditions, are assumed to be constant. Stress periods allow the model to simulate changes over time, such as seasonal variations in recharge or pumping.

Each stress period can include one or more-time **steps**, which control the numerical accuracy of the solution within the stress period.

Stress periods inserted in Transient Model

	START	LENGTH	NO OF TIME STEPS	MULTIPLIER	MAX TRANS STEPS
	01-01-2022 00:00	365	5	10	1000
	01-01-2023 00:00	365	5	10	1000
	01-01-2024 00:00	366	5	10	1000
	01-01-2025 00:00	365	5	10	1000
	01-01-2026 00:00	35063	30	10	1000
	01-01-2122 00:00	1	10	10	1000
	02-01-2122 00:00	1	10	10	1000
	03-01-2122 00:00	1	10	10	1000
	04-01-2122 00:00	1	10	10	1000
	05-01-2122 00:00	1	10	10	1000
	06-01-2122 00:00	1	10	10	1000
	07-01-2122 00:00	1	10	10	1000
	08-01-2122 00:00	1	10	10	1000
	09-01-2122 00:00	1	10	10	1000

	10-01-2122 00:00	1	10	10	1000
	11-01-2122 00:00	1	10	1	1000
	12-01-2122 00:00	1	10	1	1000
	13-01-2122 00:00	1	10	1	1000
END	14-01-2122 00:00	1	10	1	1000

Table 4.4.2 Stress Periods added to Transient Model

The prerequisite data required for running the model in a transient state are initial heads and stress periods. The year is divided into 70 stress periods, i.e., 1, 2, 3, 4, 5, and 100 years. Each stress period is divided into one-time steps to have yearly heads and flow. The prediction model was run for the 1st year, 2nd year, 3rd year and 100th year.

STEP 11: ASSIGNING LAYER PROPERTIES WITH HELP OF MATERIAL ID's

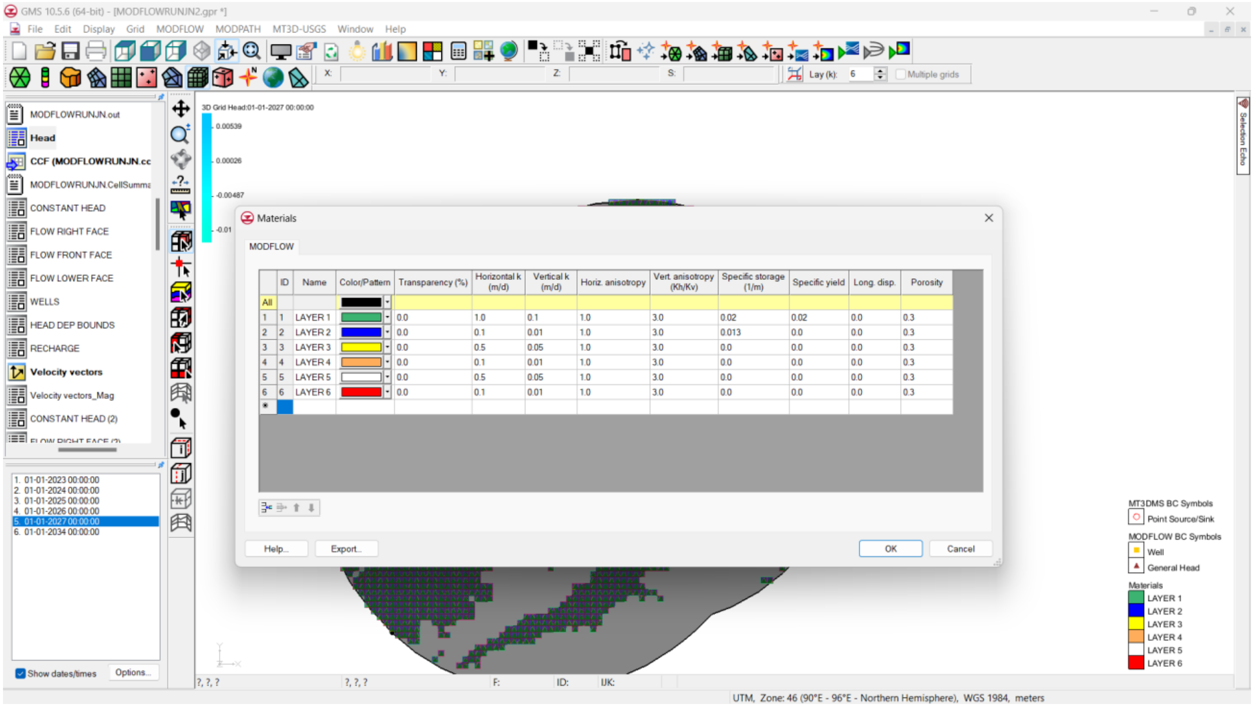


Fig 4.4.12: Assigned Layer Properties

• **Horizontal K (m/d)**: The horizontal hydraulic conductivity (K), measured in meters per day, indicates how easily water can flow horizontally through the material.

• **Vertical K (m/d)**: The vertical hydraulic conductivity, also in meters per day, measures the ease of water flow in the vertical direction.

• **Horiz.Anisotropy**: Horizontal anisotropy is the ratio of hydraulic conductivity in one horizontal direction to another (typically the x-direction compared to the y-direction).

• **Vert. Anisotropy (K_h/K_v)**: The ratio of horizontal hydraulic conductivity (K_h) to vertical hydraulic conductivity (K_v), representing how much easier water flows horizontally compared to vertically.

• **Specific Storage (1/m)**: This is the amount of water a unit volume of an aquifer releases or stores per unit change in head, expressed per meter.

• **Specific Yield**: It is the ratio of the volume of water that drains from the aquifer due to gravity to the total volume of the aquifer, representing the storage capacity in unconfined aquifers.

• **Long**. **Disp.**: Longitudinal dispersivity refers to the spreading of a solute along the flow path due to velocity variations in the pore spaces.

• **Porosity**: The fraction of the material's volume that is void space (pores), where water can be stored or move through.

STEP 12: MAP TO MODFLOW AND RUN IN TRANSIENT STATE.

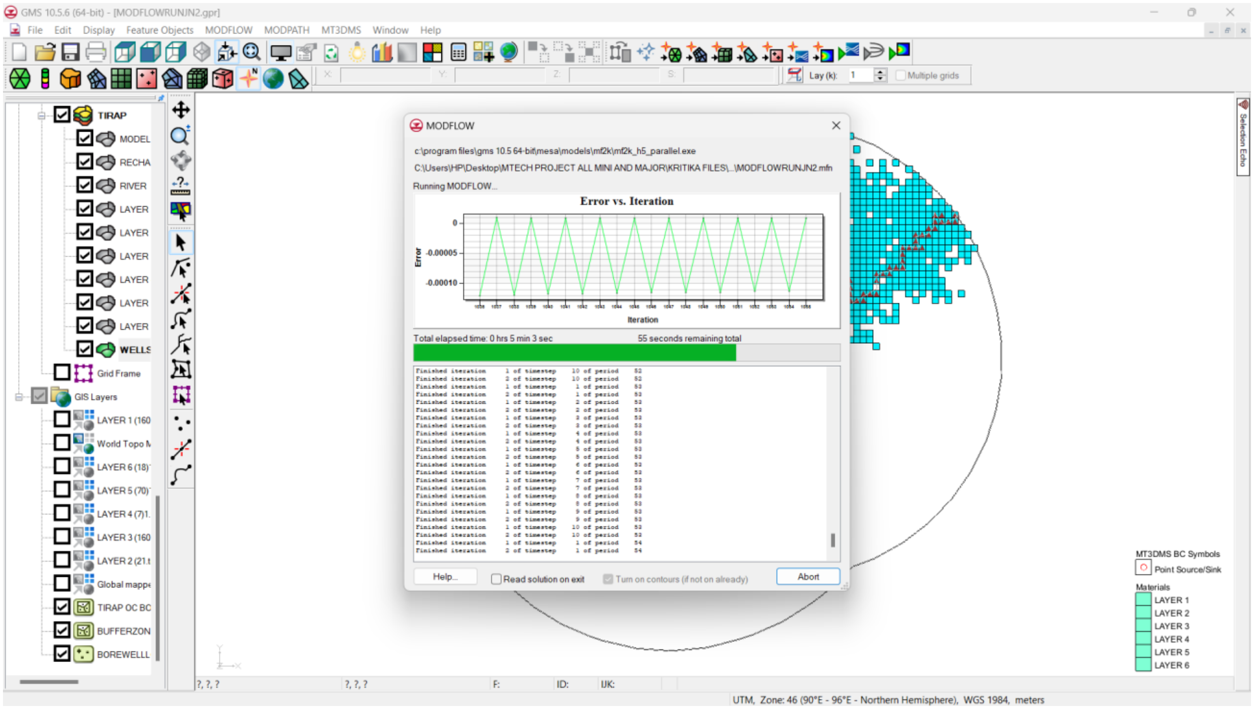
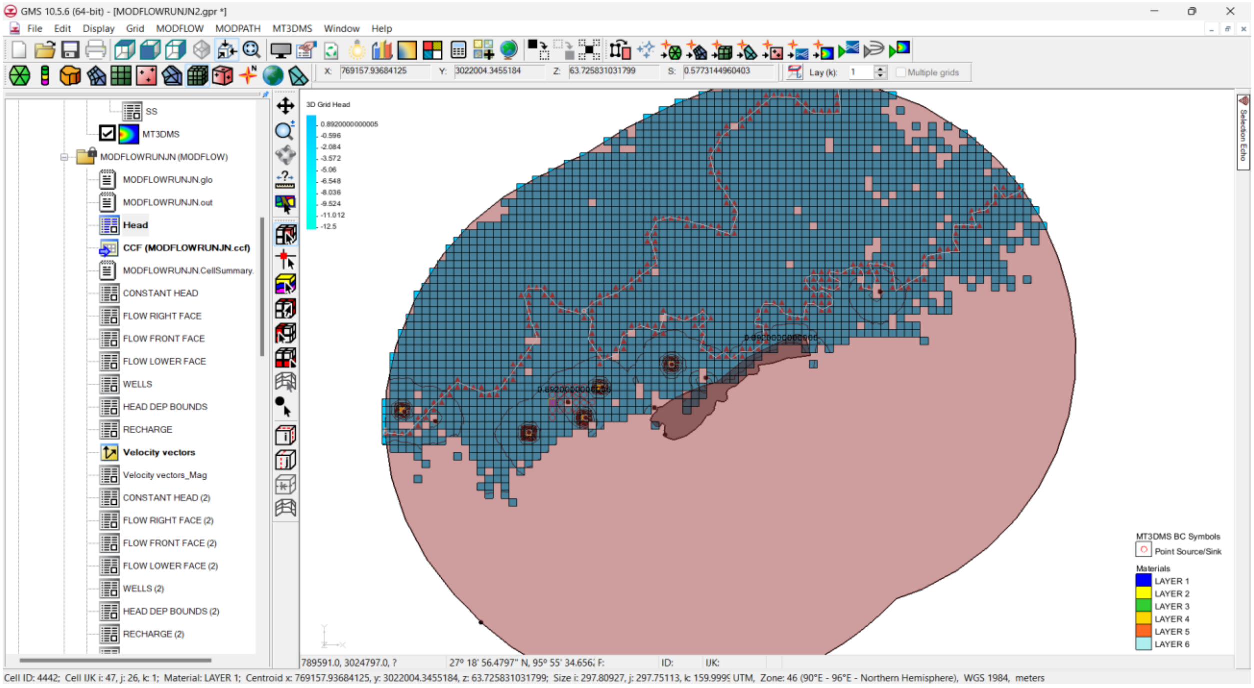


Fig 4.4.13. Running State of Transient Model where iterations are being performed.

- TOTAL RUN TIME taken 6minutes 40 seconds.
- TOTAL SUM OF SQUARED, WEIGHTED RESIDUALS = 0.405E-22 which is an extremely small value, indicating that the simulation has achieved a nearly perfect fit to the observations with almost no residual error.



The pink grid in the fig 4.4.14 represents inactive area as the region is hilly.

STEP 13: CALIBRATION OF TRANSIENT MODEL.

a) Entering Recharge Rate CSV file for years to be predicted (recharge rate was assumed for other years)

YEARS	RECHARGE RATE
01-01-2022	0.000624
01-01-2023	0.000752
01-01-2024	0.000452
01-01-2025	0.000704
01-01-2026	0.000665
01-01-2122	0.000665

Table 4.4.3: Year vs Recharge rate data for transient calibration

b) Entered Bore Well Data with a Start and End date (pumping data was assumed)

Table 4.4.5: Bore well flow rate data with start and end date.

WELLS	START DATE	FLOW RATE (M^2/day)
BW-1	01-01-2021	-500
BW-1	01-01-2122	0
BW-2	01-01-2021	-500
BW-2	01-01-2122	0
BW-3	01-01-2021	-500
BW-3	01-01-2122	0
BW-4	01-01-2021	-500
BW-4	01-01-2122	0
BW-5	01-01-2021	-500
BW-5	01-01-2122	0
BW-6	01-01-2021	-500
BW-6	01-01-2122	0
BW-7	01-01-2021	-500
BW-7	01-01-2122	0
BW-8	01-01-2021	-500
BW-8	01-01-2122	0
BW-9	01-01-2021	-500
BW-9	01-01-2122	0

STEP 14: TRANSIENT MODEL AFTER CALIBRATION.

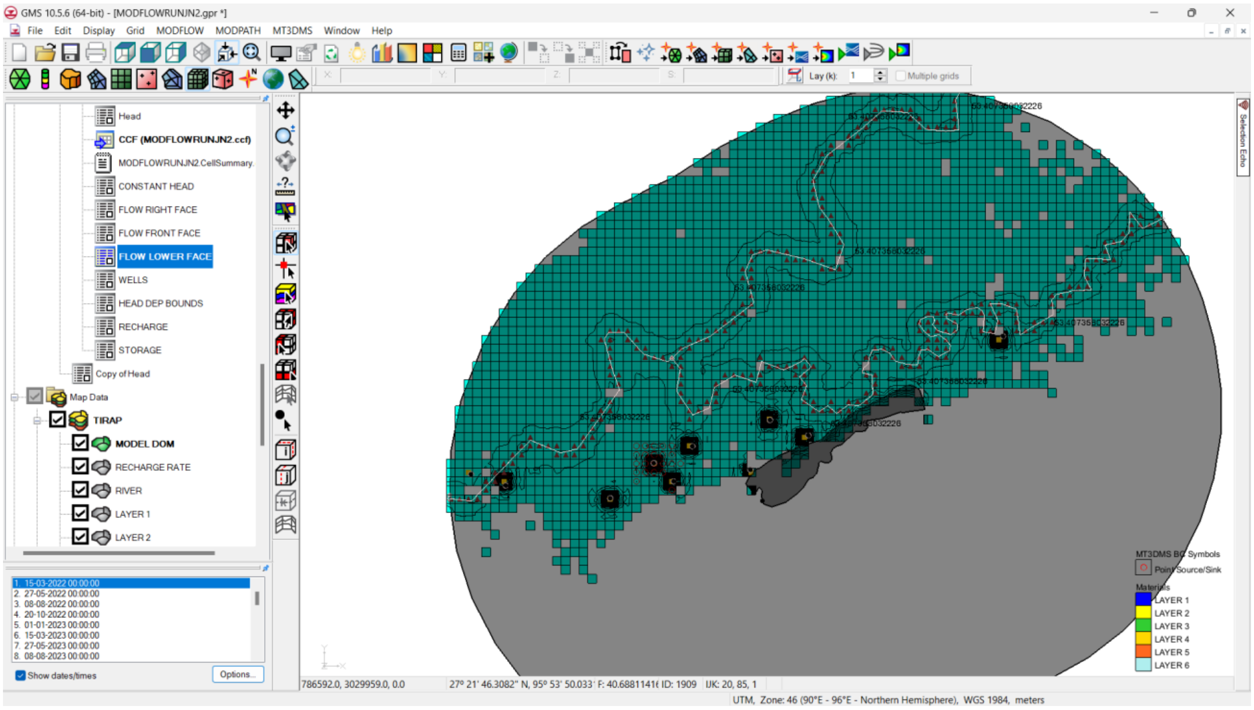


Fig 4.4.15: Transient Model after calibration

In the fig 4.4.15 following things can be viewed.

- **Main View Area**:

The central area shows a grid-based model with coloured cells, representing layers of a hydrogeological model. The grid indicates spatial discretization for the model. Different colors on the grid (e.g., blue, gray, green) represents different layers or zones with distinct properties.

- **Layer Information and Components (left panel):**

The hierarchical panel shows the components of the model. It includes datasets such as "CONSTANT HEAD," "FLOW FRONT FACE," "RECHARGE," and "STORAGE," which are of a MODFLOW simulation. Specific layers (Layer 1-60 and other elements like "RIVER" and "RECHARGE RATE" are also visible, indicating groundwater interactions and recharge zones.

- **Temporal Data (bottom left):**

A timeline section shows simulation dates for running different time steps or scenarios.

STEP 15: ADDING MT3DMS TO MODFLOW.

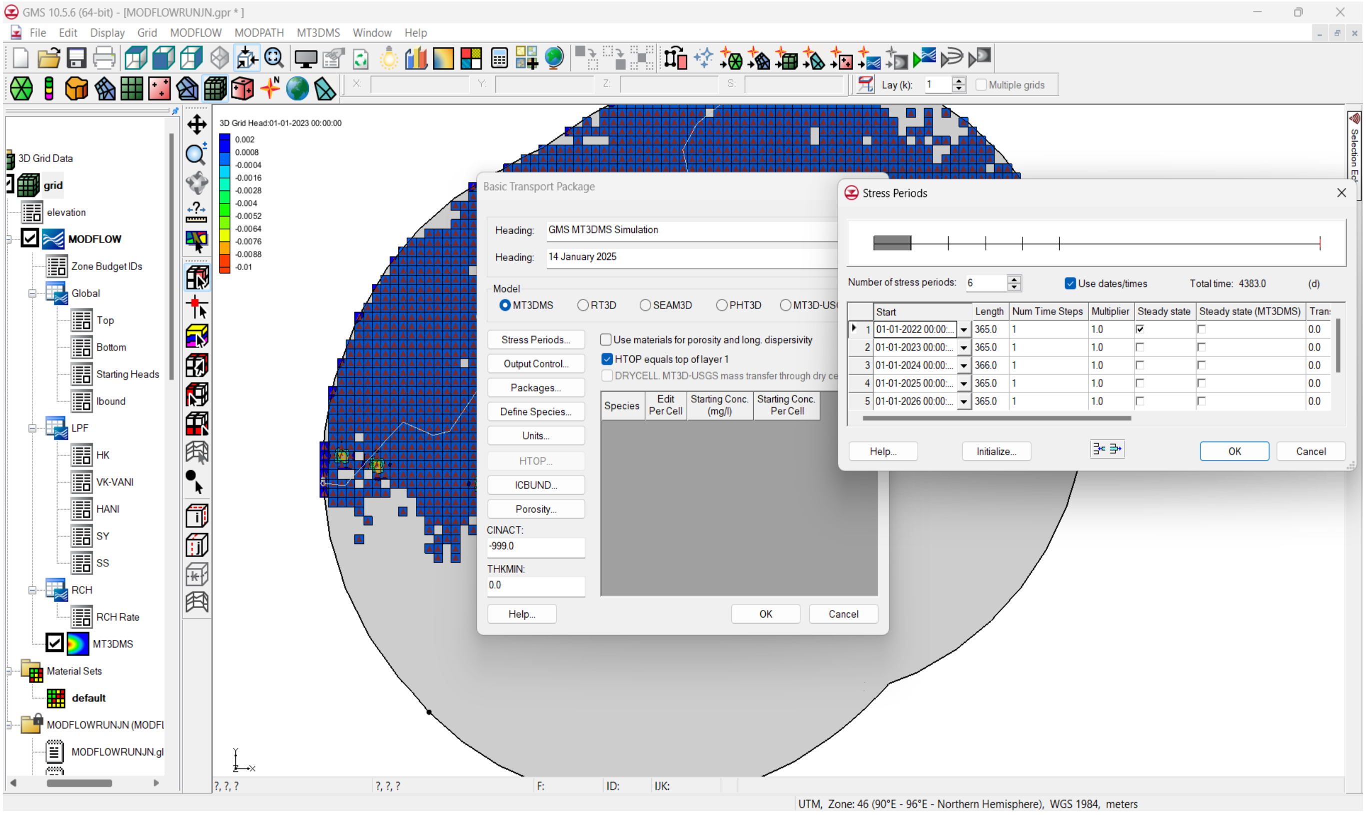


Fig 4.4.16: First approach towards MT3DMS

MT3DMS is a multi-species model, so first we need to define the number of species and name each one. In this case, there is only one species and name it as Contaminant and then add stress periods same as in the transient model.

MT3DMS (Modular Three-Dimensional Multi-Species Transport Model) is a widely used numerical modeling software designed to simulate the transport of contaminants in groundwater systems. It works as an extension to the groundwater flow model MODFLOW and relies on its flow solution to calculate advection, dispersion, and chemical reactions of dissolved contaminants in groundwater. Developed originally by Chunmiao Zheng in the early 1990s, MT3DMS has become a standard tool for studying groundwater contaminant transport.

STEP 16: SELECTING DIFFERENT PACKAGES

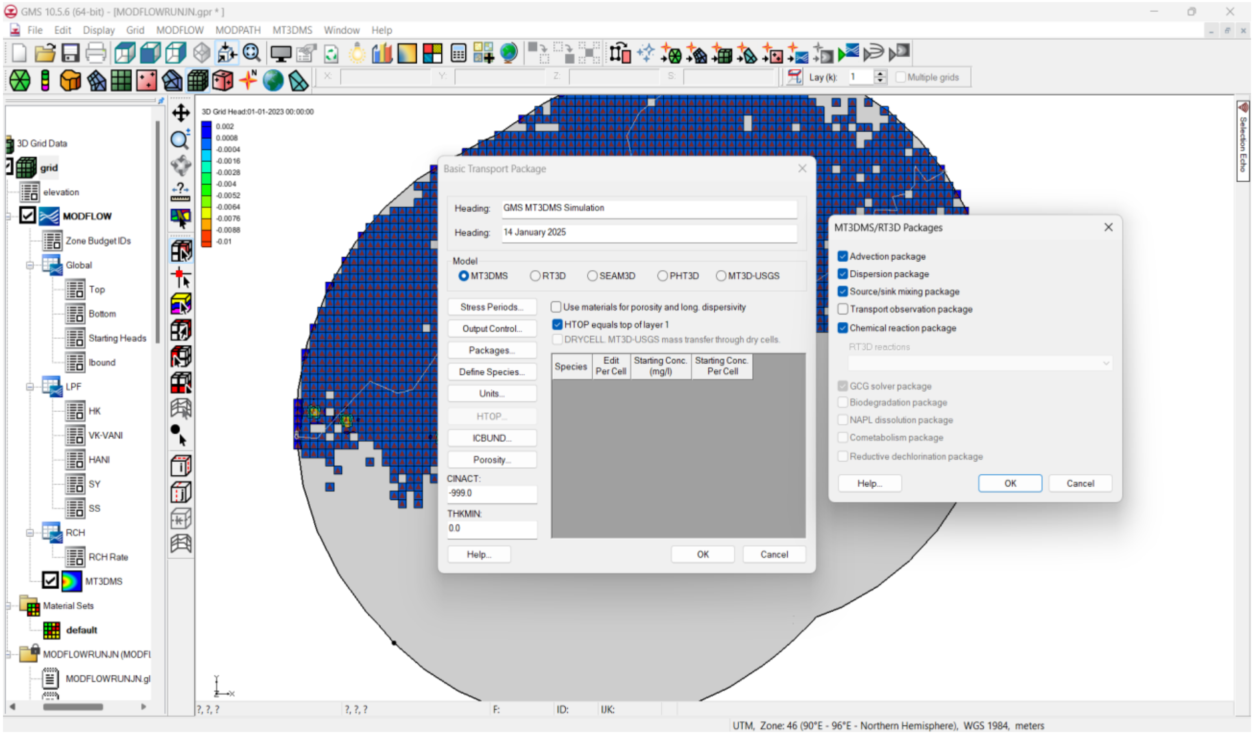


Fig 4.4.17: Package Selection

The Advection-Dispersion-Chemical Reaction (ADCR) package is a critical module in groundwater modelling, designed to simulate the transport and transformation of chemical constituents within groundwater systems. It integrates processes such as advection, dispersion, and chemical reactions to model how contaminants or nutrients migrate through subsurface environments. This package is particularly important for understanding pollution transport, nutrient cycling, and contaminant degradation in groundwater systems.

- **Advection**

  Advection refers to the movement of dissolved chemicals due to the bulk motion of groundwater. It is driven by hydraulic gradients and follows Darcy's law, which describes the flow of groundwater through porous media. In the ADCR package, advection is modeled by solving equations that describe the movement of solutes along the flow field. This process ensures that solutes are transported in accordance with the velocity and direction of groundwater flow.

- **Dispersion**

  Dispersion accounts for the spreading of solutes due to variations in flow velocities within the pore spaces of the aquifer. It includes both mechanical dispersions,9 caused by differences in flow paths and velocities, and molecular diffusion, which results from the random movement of solute molecules. The

ADCR package incorporates these effects using mathematical formulations that capture the mixing and spreading of solutes as they move through the groundwater system.

- **Chemical Reactions**

  Chemical reactions in the ADCR package cover a wide range of processes, including sorption, precipitation, dissolution, and redox reactions. These reactions influence the concentration and mobility of chemical species in groundwater. The package uses reaction kinetics and equilibrium models to simulate these processes. It can handle single-species reactions as well as complex multi-species interactions, making it a powerful tool for predicting the fate of reactive contaminants.

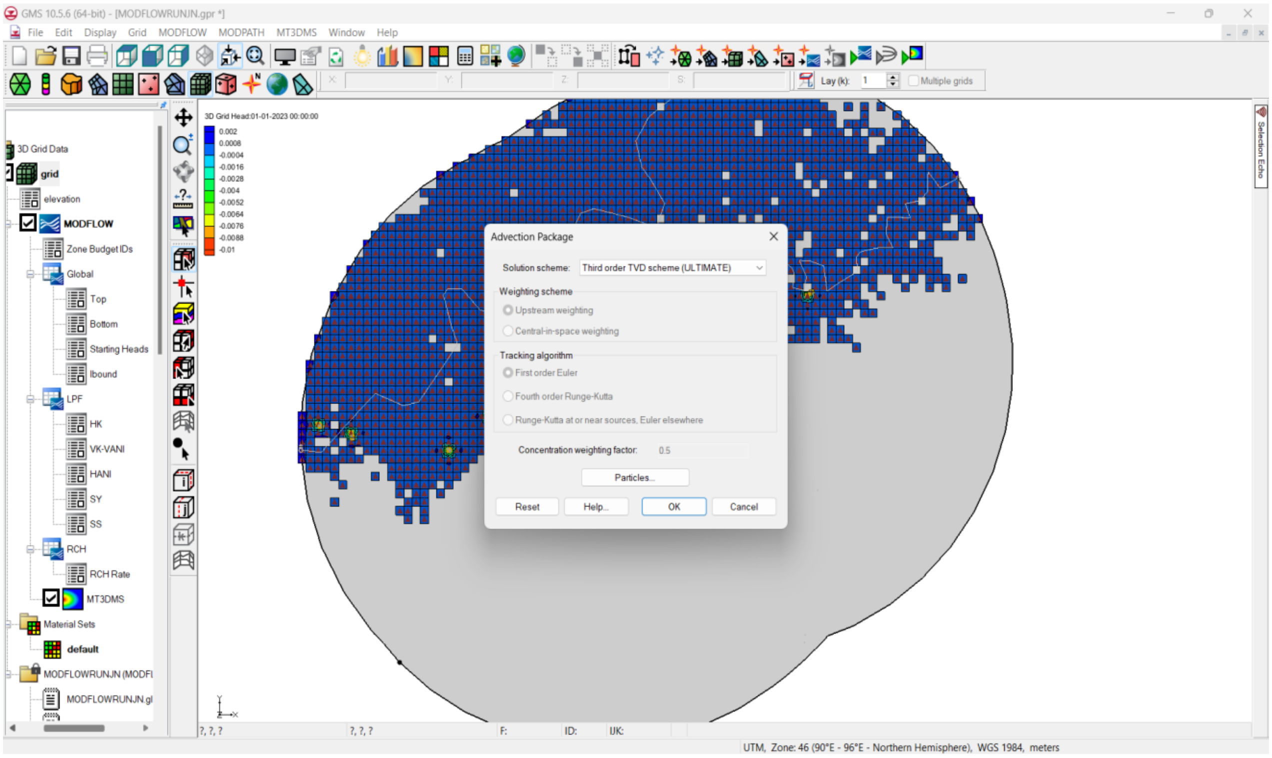


Fig 4..4.18 Advection Package

In this Fig 16.1 i. e in the Advection package the TVD scheme is used which is a type of higher-order numerical method used in solving advection-dominated transport problems. It minimizes numerical dispersion and oscillations, ensuring stability and accuracy in the solution.

- **Total Variation Diminishing (TVD)**: This means the numerical method ensures that the "total variation" (a measure of oscillations in the solution) does not increase as the simulation progresses. This helps prevent spurious oscillations (artificial fluctuations in concentration values).
- **Third Order:** Refers to the accuracy of the scheme. A third-order scheme provides higher accuracy in resolving sharp concentration gradients (e.g., contaminant fronts) compared to first- or second-order methods.

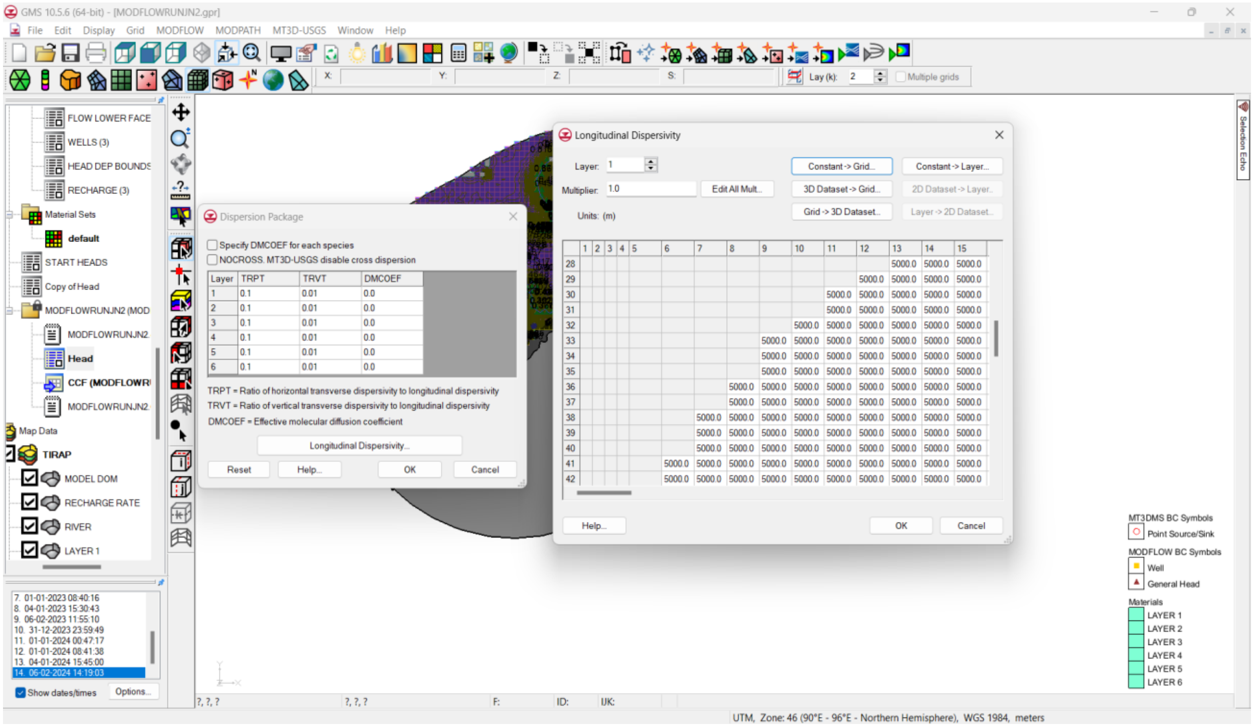


Fig 4.4.19 Dispersion Package

- In this Fig 4.4.19 TRP 1 represents the transverse dispersivity in the horizontal direction, perpendicular to the primary flow direction. It describes the extent to which solutes spread laterally due to mechanical dispersion. This parameter accounts for the spreading of solutes in the horizontal plane as they move through porous media. It is essential for capturing the realistic plume behavior, especially in heterogeneous aquifers. Typically measured in length units (e.g., meters or feet)

- TRVT refers to the transverse dispersivity in the vertical direction, perpendicular to both the flow direction and the horizontal plane. This parameter models solute spreading vertically due to dispersion. TRVT is crucial for understanding the vertical mixing of solutes, particularly in scenarios involving vertical gradients, such as contaminant migration through layered aquifers or to/from confining units. Typically measured in length units (e.g., meters or feet)

- DMCOEF represents the molecular diffusion coefficient, which quantifies the rate of solute diffusion at the molecular level due to concentration gradients. This parameter captures the solute movement due to molecular diffusion, independent of bulk groundwater motion. While typically smaller than mechanical dispersion in many groundwater systems, molecular diffusion can dominate in low-velocity or stagnant zones. Measured in units of area per time (e.g., m^2/s or ft^2/day).

- **Longitudinal dispersivity** quantifies the degree to which a solute plume elongates in the direction of flow because of velocity variations at the pore scale.It is influenced by the heterogeneity of the aquifer material and the flow velocity. In simple terms, it accounts for the differences in flow paths and speeds encountered by water particles as they pass through an aquifer.

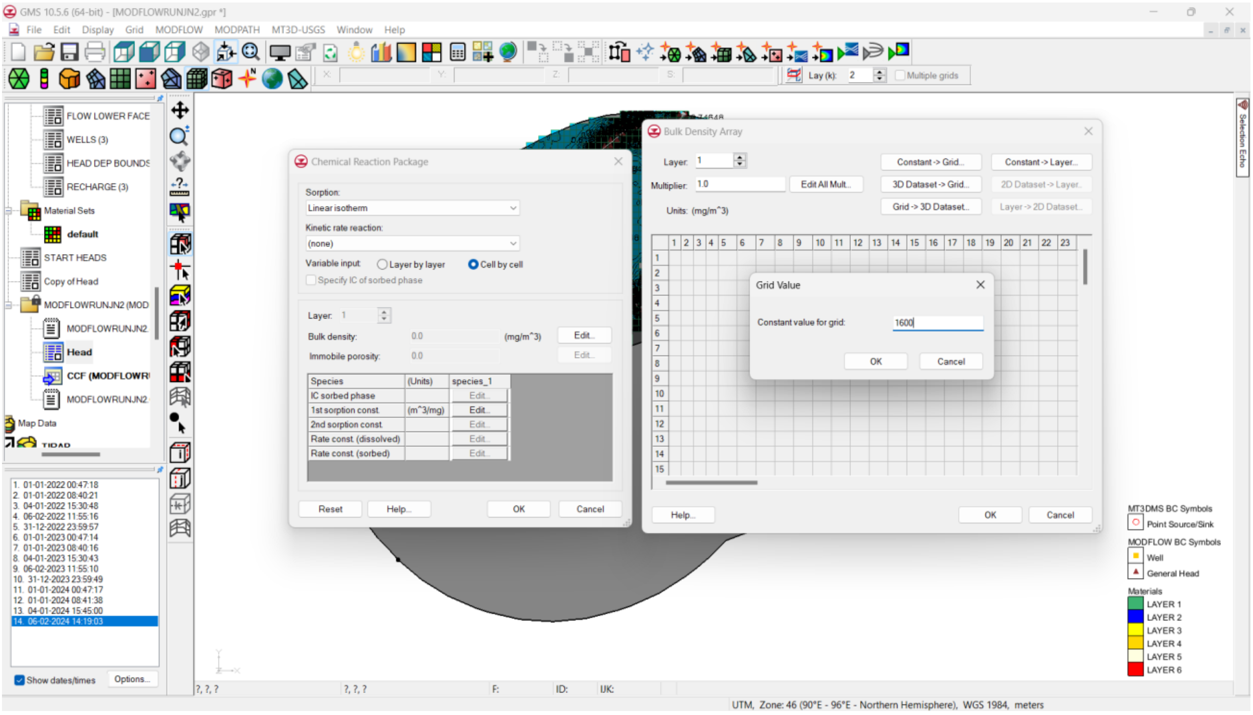


Fig 4.4.20 Chemical Reaction Package

In this fig 4.4.20 A **linear isotherm** sorption was taken as it is one of the simplest models for representing sorption processes, where the amount of solute sorbed to the solid phase is directly proportional to the solute concentration in the aqueous phase. The relationship can be expressed as:

$$S=K_d \cdot C \quad \text{where,}$$

- S: Sorbed concentration (mass of solute per unit mass of solid).
- K_d: Distribution coefficient (represents the sorption capacity of the solid).
- C: Solute concentration in the aqueous phase
- Bulk density in Chemical reaction package is the total mass of the solute in the system includes both the dissolved phase in the water and the sorbed phase on the solid. Bulk density is used to convert the solid-phase sorption (mass per unit mass of solids) into a volumetric term that matches the aqueous phase (mass per unit volume of water).

- The total concentration of solute in the system (C_t) is given by:

$$C_t = C + (\rho b/\theta) * SC$$

In this model we assumed the bulk density to be 1600

STEP 17 :TURNING ON TRANSPORT IN TIRAP AND DEFINE THE SPECIES AGAIN

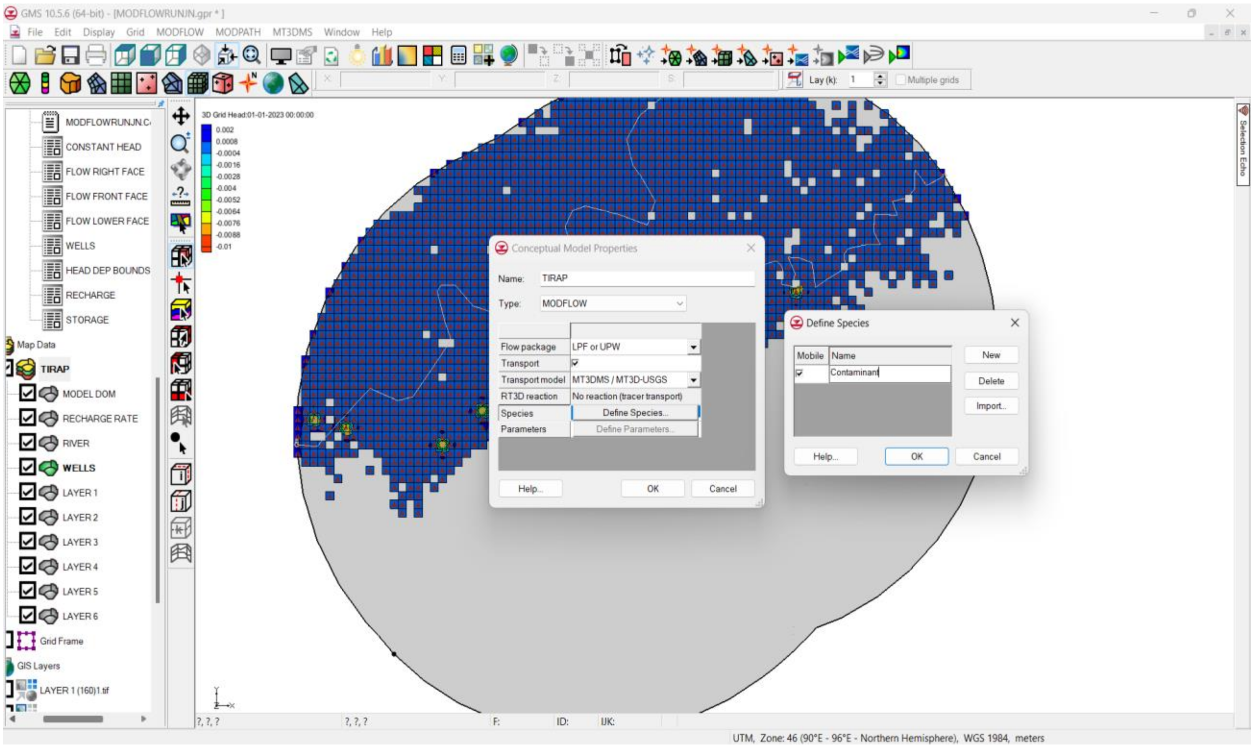


Fig 4.4.21: Assigning properties in Tirap

In the Tirap conceptual model properties were changed to transport and species was defined again as a contaminant.

STEP 18: CREATING NEW COVERAGE FOR SOURCE CONCENTRATION

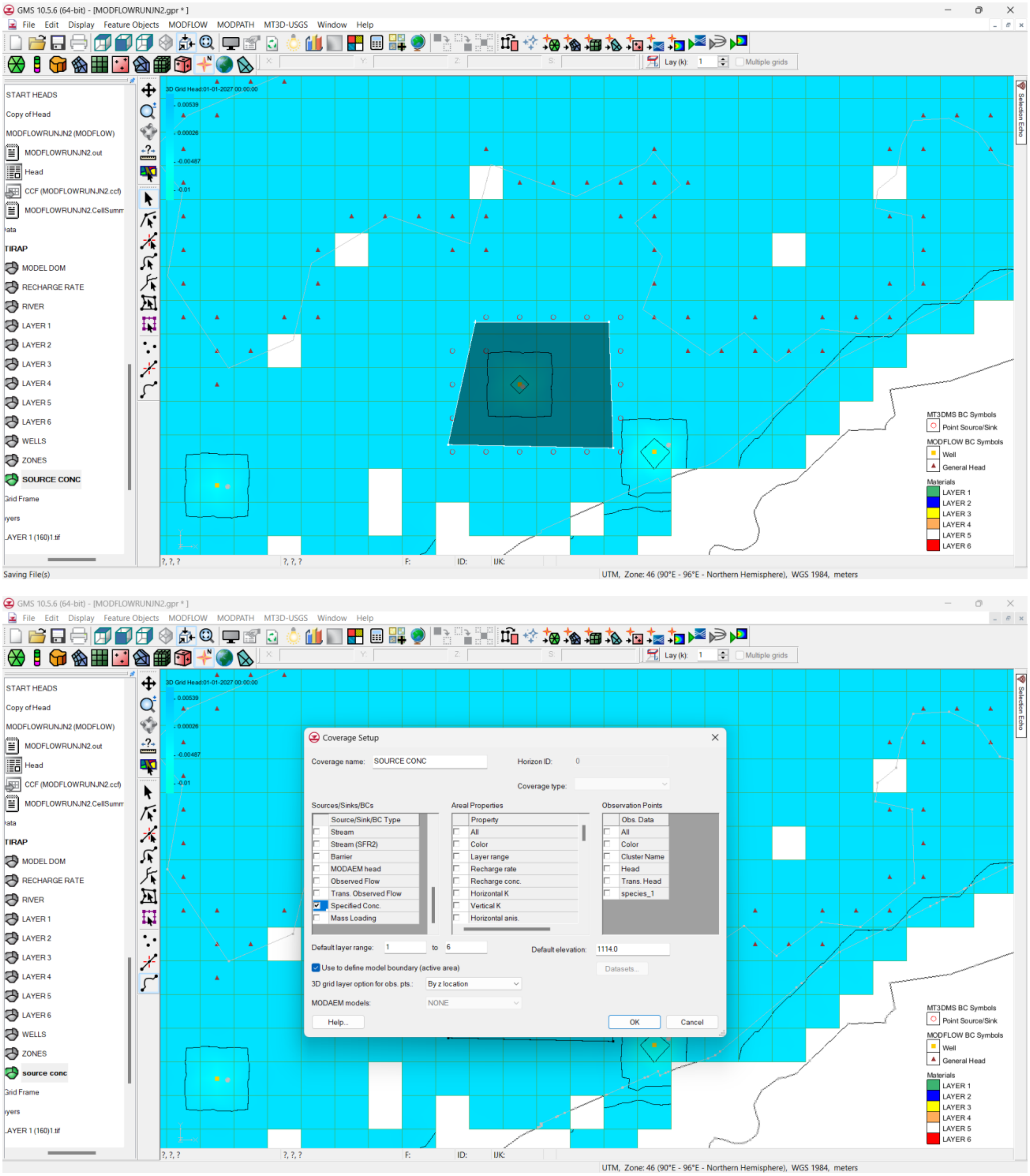


Fig 4.4.22: New polygon created for Source Concentration.

After these steps the coverages were mapped to MODFLOW and MT3DMS and then started

The MT3DMS FILE WAS ABORTED

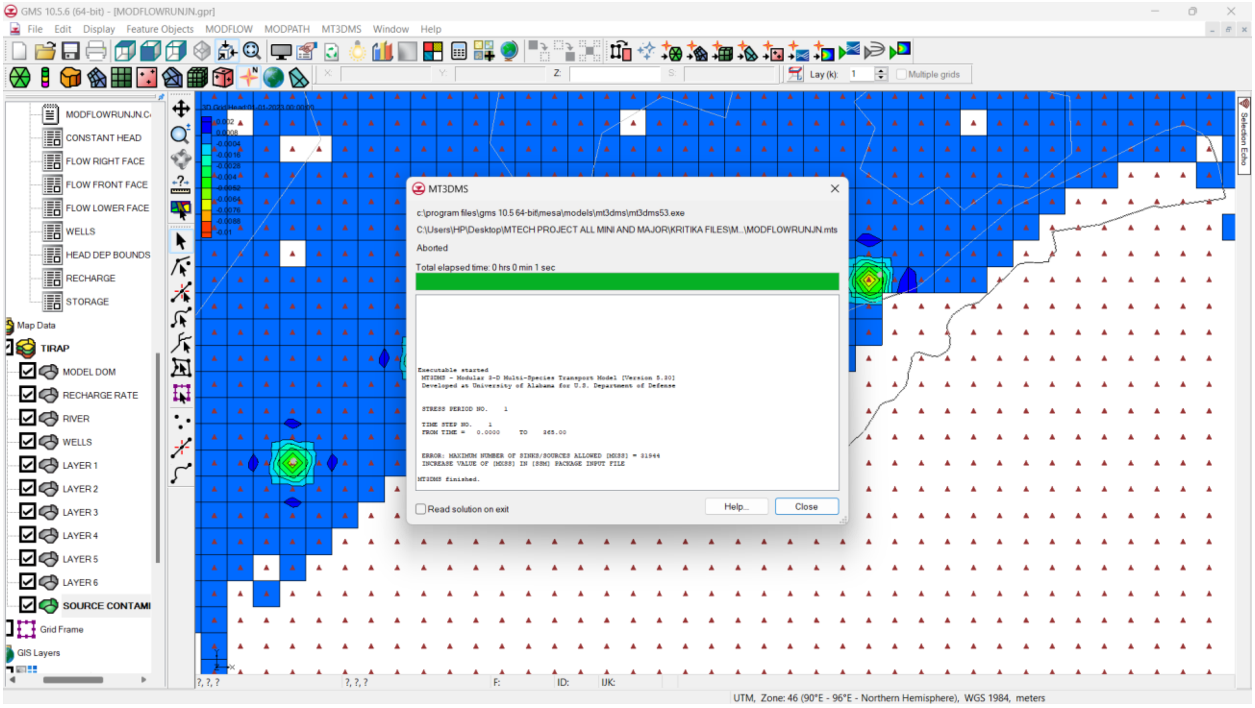


Fig 4.4.23: Aborted MT3DMS

Cause of the Error: The number of sources/sinks in this model might exceeds the maximum limit defined by the current value of `DOBS` in the input file (11004 in this case). This limit restricts the total number of active sources/sinks .

4.5 TRIAL FOR MT3DMS IN ANOTHER WAY

As the MT3DMS file was aborted another attempt for MODFLOW was done in Steady state with the same methodology considering only 1 layer having default elevation as 0.

- **Step 1 -**
  - Setting up MODFLOW model to define heads and flows
- **Step 2 -**

Add MT3DMS to Project Explorer/Model Interfaces, activate it in Model Properties

MT3DMS: new simulation

Basic Transport Package -

- Output Control:
- Packages: Advection, Dispersion, Chemical Reaction
- Define Species TCE (TRI CHOLRO ETHYLENE)
- MT3DMS stress period = 50 yrs ~1.5E9s, multiplier = 1.03, max timestep=1E6s
- Assume the flow is steady state
- Porosity-0.1
- Advection Package: use as default
- Dispersion Package
- Long. Dispersivity = 20 ft, defaults on transverse etc. (TRPT, TRVT, DMCOEF)
- Chemical Reaction Package: Linear isotherm, variable input: Cell by cell.
- bulk density=1.6 gm/ml; Kd=0.1 ml/gm

- **Step 3**
  - Map Data → Model → Properties
  - Check transport box, define species → name must match earlier definition
  - Adding Coverage
  -
  - Coverage set up → source/sink/BC→ Selected specified conc.
  - Draw locations of sources as polygons,
  - specify concentration=1000 mg/L
- **Step 4**
  - Map coverage → MT3DMS
  - Check MT3D (optional)
  - Run MT3D
- **Step 5**
  - Plume maps at different times and layers
  - 3D in Perspective view.

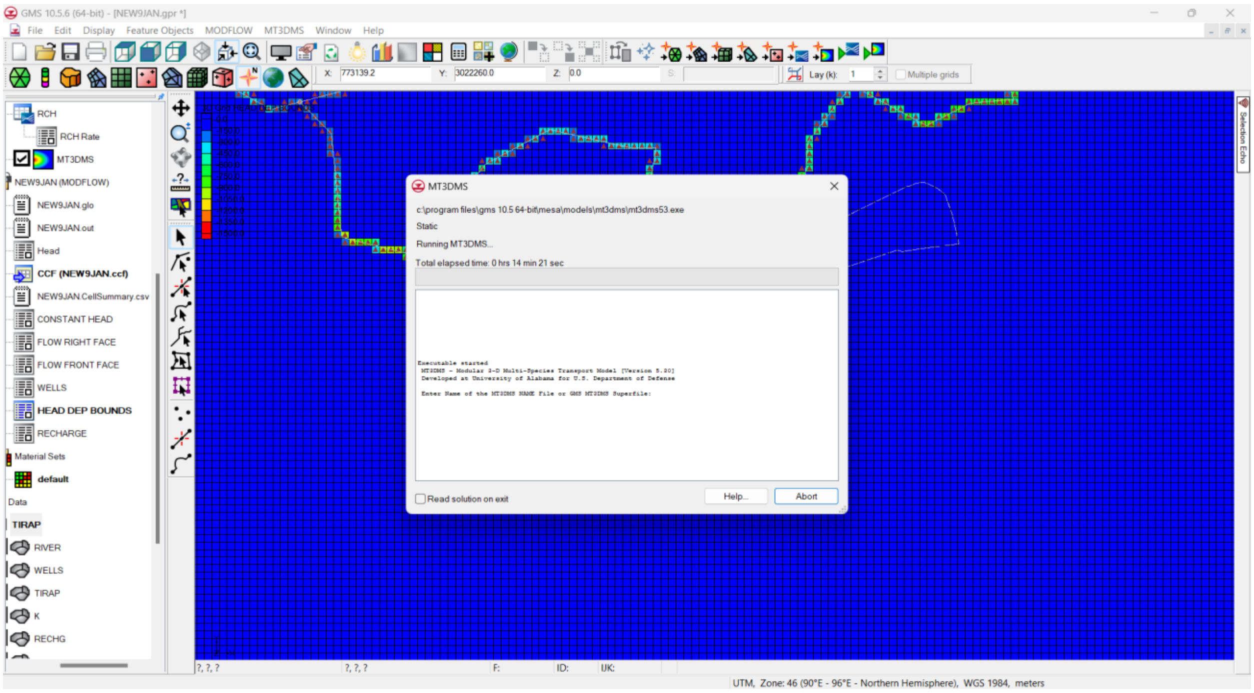


Fig 4.4.24: Aborted in Steady state considering single layer.

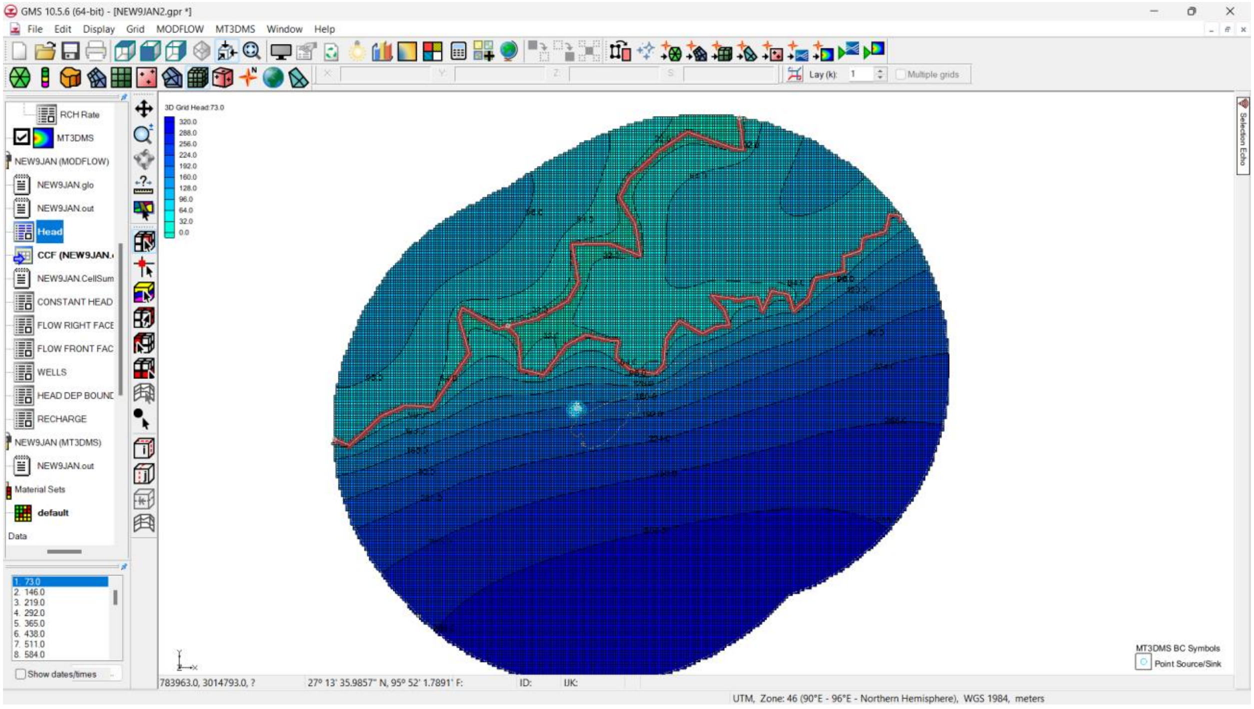


Fig 4.4.25: After the MT3DMS is aborted the model is displayed in this manner

5. RESULTS AND DISCUSSIONS

5.1 TRANSIENT SIMULATION FLOW BUDGET

5.1.1. LAYER 1 Flow budget for year 2022,

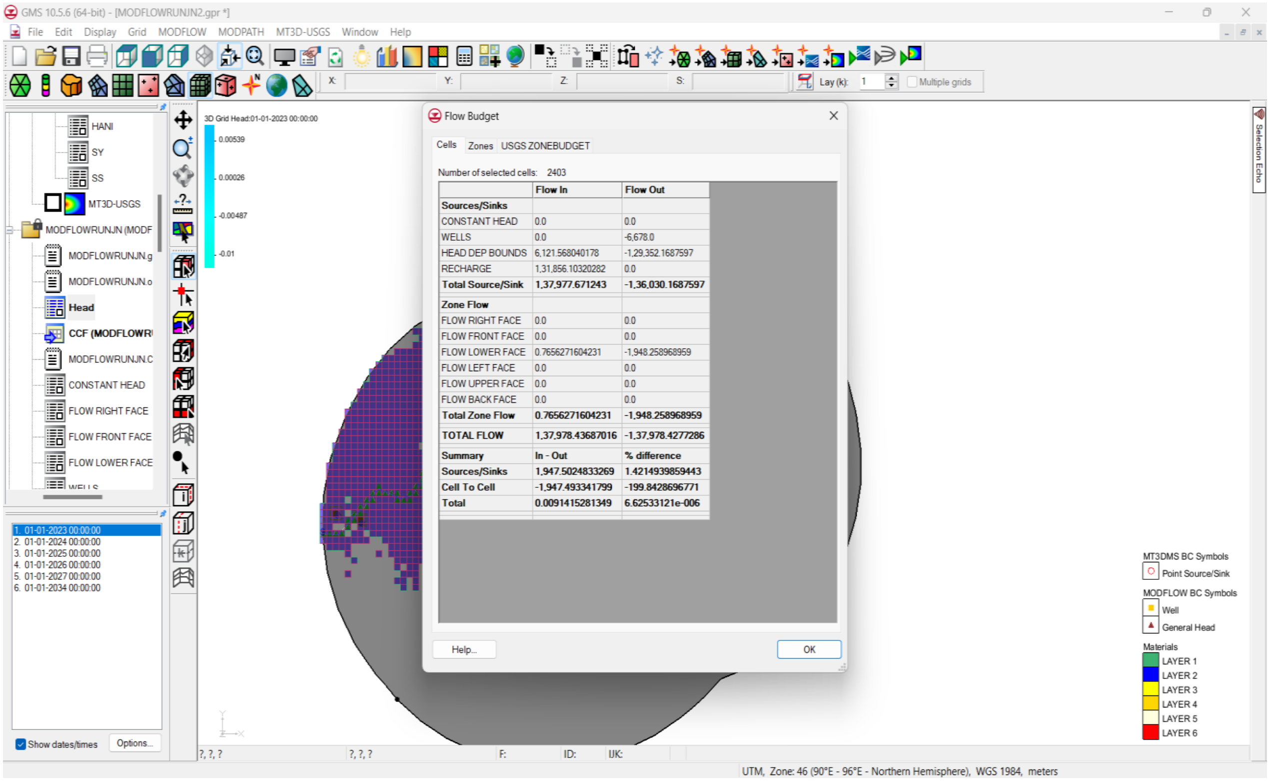


Fig 5.1 Layer 1 Flow budget

Sources/Sinks	**Flow In**	**Flow Out**	**REMARKS**
CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
WELLS	0	-6.678	Wells act as a sink, with water extraction of 6.678 units.
HEAD DEP BOUNDS	6.1216	-129.356	Dynamic inflow and outflow interaction with external boundaries.
RECHARGE	1,318.86	0	Recharge adds water to the system, purely inflow.
TOTAL Source/Sink	1,379.98	-1,360.17	Net inflow from all sources and sinks is positive.
Zone Flow			

FLOW RIGHT FACE	0	0	No flow occurred through this boundary.
FLOW FRONT FACE	0	0	No flow occurred through this boundary.
FLOW LEFT FACE	0	0	No flow occurred through this boundary.
FLOW BACK FACE	0	0	No flow occurred through this boundary.
FLOW LOWER FACE	0.7656	-1.9483	Small inflow and outflow occurred across the lower boundary face.
FLOW UPPER FACE	0	0	No flow occurred through the upper boundary.
TOTAL Zone Flow	0.7656	-1.9483	Net outflow across the zone boundaries.
TOTAL FLOW	1,379.98	-1,379.98	Total inflow matches outflow, satisfying the mass balance principle.
Summary			
Sources/Sinks (In/Out)	1,947.50	-1,421.49	Summarizes flow due to sources and sinks, with no major discrepancies.
Cell-To-Cell Flow (In/Out)	-1,947.49	199.8428	Cell-to-cell flow is consistent with minimal difference, ensuring mass balance.
Total Difference	0.0091	-6.63E-06	Extremely small differences validate that mass is conserved

Table 5.1 Layer 1 flow budget for transient

Interpretation:

- **Recharge** is the primary inflow into the system (1318.86 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model.

5.1.2 Layer 2 Flow Budget

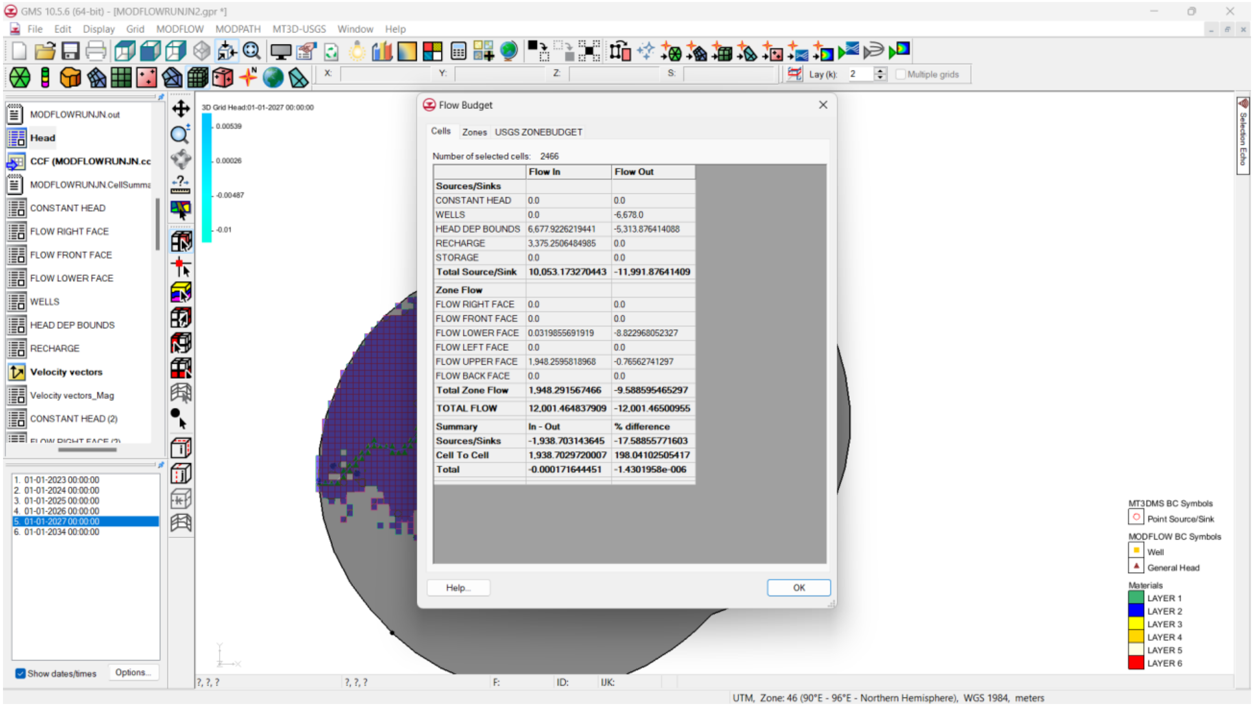


Fig 5.2: Layer 2 Flow budget

Sources/Sinks	**FLOW IN**	**FLOW OUT**	
CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
WELLS	0	-6,678.00	Wells act as a sink, with water extraction of 6.678 units.
HEAD DEP BOUNDS	6,677.92	-5,313.88	Dynamic inflow and outflow interaction with external boundaries.
RECHARGE	3,375.25	0	Recharge adds water to the system, purely inflow.
Total Source/Sink	10,053.17	-11,991.88	Net inflow from all sources and sinks is positive.
Zone Flow			
FLOW RIGHT FACE	0	0	No flow occurred through this boundary.

FLOW FRONT FACE	0	0	No flow occurred through this boundary.
FLOW LOWER FACE	0.031985569	-8.822968052	Small inflow and outflow occurred across the lower boundary face.
FLOW LEFT FACE	0	0	No flow occurred through this boundary.
FLOW UPPER FACE	1,948.26	-0.765627413	Small inflow and outflow occurred across the lower boundary face.
FLOW BACK FACE	0	0	No flow occurred through the upper boundary.
Total Zone Flow	1,948.29	-9.588595465	Net outflow across the zone boundaries.
TOTAL FLOW	12,001.46	-12,001.47	Total inflow matches outflow, satisfying the mass balance principle.
Summary	In - Out	% difference	
Sources/Sinks	-1,938.70	-17.58855772	Summarizes flow due to sources and sinks, with no major discrepancies.
Cell To Cell	1,938.70	198.0410251	Cell-to-cell flow is consistent with minimal difference, ensuring mass balance.
Total	-0.000171644	-1.43E-06	Extremely small differences validate that mass is conserved
Sources/Sinks	-1,938.70	-17.58855772	Summarizes flow due to sources and sinks, with no major discrepancies.

Table 5.2 Layer 2 flow budget for transient simulated model

Interpretation:

- **Recharge** is the primary inflow into the system (3,375.25 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model

5.1.3 Layer 3 Flow Budget

Category	Component	Flow In	Flow Out	Remarks
Sources/Sinks	Constant Head	0	0	No contribution from constant head.
	Wells	0	-6.678	Water extraction from wells (outflow).
	Head Dep Bounds	6.676693657	-75.748755	Significant inflow and outflow due to head-dependent boundaries.
	Recharge	75,694.15	0	Major inflow source from recharge.
	Storage	0	0	No storage contribution.
	Total Source/Sink	82,370.84	-82,165.55	Net flow from sources and sinks.
Zone Flow	Flow Right Face	0	0	Negligible flow across the right face.
	Flow Front Face	0	0	Negligible flow across the front face.
	Flow Lower Face	0.026411693	-214.10948	Small inflow but significant outflow across the lower face
	Flow Left Face	0	0	No flow across the left face.

	Flow Upper Face	8.822968052	-0.0031986	Noticeable inflow with negligible outflow across the upper face.
	Flow Back Face	0	0	No flow across the back face.
	Total Zone Flow	8.849379745	-214.14147	Total inflow and outflow across all faces.
Total Flow	(Combined)	82,379.69	-82,379.69	Sum of total inflow and total outflow across sources, sinks, and faces.
Summary	Sources/Sinks In - Out	205.2921533		Difference in flow balance from sources and sinks.
	Cell-to-Cell Flow	-205.2920948		Balances flow internally between cells.

Table 5.3 Layer 3 flow budget for transient simulated model

Interpretation:

- **Recharge** is the primary inflow into the system (75,694 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model

5.1.4 Layer 4 Flow Budget

Sources/Sinks	FLOW IN	FLOW OUT	REMARKS
CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
WELLS	0	-6,678.00	Wells act as a sink, with water extraction of 6.678 units.
HEAD DEP BOUNDS	6,677.99	-2,971.24	Dynamic inflow and outflow interaction with external boundaries.
RECHARGE	2,766.60	0.00	Recharge adds water to the system, purely inflow.
STORAGE	0	0	
Total Source/Sink	9,444.59	-9,649.24	Net inflow from all sources and sinks is positive.
Zone Flow			
FLOW RIGHT FACE	0	0	No flow occurred through this boundary.
FLOW FRONT FACE	0	0	No flow occurred through this boundary.
FLOW LOWER FACE	0.019762117	-9.457717842	No flow occurred through this boundary.
FLOW LEFT FACE	0	0	No flow occurred through this boundary.
FLOW UPPER FACE	214.1094846	-0.026411693	Small inflow and outflow occurred across the lower boundary face.
FLOW BACK FACE	0	0	No flow occurred through the upper boundary.
Total Zone Flow	214.1292467	-9.48	Net outflow across the zone boundaries.
TOTAL FLOW	9,658.72	-9,658.72	Total inflow matches outflow, satisfying the mass balance principle.
Summary	In - Out	% difference	
Sources/Sinks	-204.6452164	-2.143574148	Summarizes flow due to sources and sinks, with no major discrepancies.

Cell To Cell	204.6451172	183.0347724	Cell-to-cell flow is consistent with minimal difference ensuring mass balance.
Total	-9.91895E-05	-1.03E-06	Extremely small differences validate that mass is conserved.

Table 5.4 Layer 4 flow budget for transient simulated model

Interpretation:

- **Recharge** is the primary inflow into the system (2,766.60 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model

5.1.5 LAYER 5 Flow Budget

SOURCES/SINKS	FLOW IN	FLOW OUT	REMARKS
CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
WELLS	0	-6,678.00	Wells act as a sink, with water extraction of 6.678 units.
HEAD DEP BOUNDS	6,679.05	-24,135.64	Dynamic inflow and outflow interaction with external boundaries.
RECHARGE	24,180.07	0	Recharge adds water to the system, purely inflow.
STORAGE	0	0	
Total Source/Sink	30,859.12	-30,813.64	Net inflow from all sources and sinks is positive.
ZONE FLOW			
FLOW RIGHT FACE	0	0	No flow occurred through this boundary.
FLOW FRONT FACE	0	0	No flow occurred through this boundary.
FLOW LOWER FACE	0.0142105	-54.93015978	No flow occurred through this boundary.
FLOW LEFT FAC	0	0	No flow occurred through this boundary.

FLOW UPPER FACE	9.457717842	-0.019762117	Small inflow and outflow occurred across the lower boundary face.
FLOW BACK FACE	0	0	No flow occurred through the upper boundary.
Total Zone Flow	9.471928342	-54.94992189	Net outflow across the zone boundaries.
TOTAL FLOW	30,868.59	-30,868.59	Total inflow matches outflow, satisfying the mass balance principle.
Summary	In - Out	% difference	
Sources/Sinks	45.4778998	0.147481311	Summarizes flow due to sources and sinks, with no major discrepancies.
Cell To Cell	-45.47799355	-141.1881012	Cell-to-cell flow is consistent with minimal difference, ensuring mass balance.
Total	-0.00009375	-3.07E-07	Extremely small differences validate that mass is conserved.

Table 5.5 Layer 5 flow budget for transient simulated model

Interpretation:

- **Recharge** is the primary inflow into the system (24,180.07 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model.

5.1.6 Layer 6 Flow Budget

Sources/Sinks	Flow In	Flow out	Remarks
CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
WELLS	0	-6,678.00	Wells act as a sink, with water extraction of 6.678 units.
HEAD DEP BOUNDS	6,676.95	-4,812.42	Dynamic inflow and outflow interaction with external boundaries.
RECHARGE	4,758.55	0	Recharge adds water to the system, purely inflow.
STORAGE	0	0	
Total Source/Sink	11,435.50	-11,490.42	Net inflow from all sources and sinks is positive.
Zone Flow			
FLOW RIGHT FACE	0	0	No flow occurred through this boundary.
FLOW FRONT FACE	0	0	No flow occurred through this boundary.
FLOW LOWER FACE	0	0	No flow occurred through this boundary.
FLOW LEFT FACE	0	0	No flow occurred through this boundary.
FLOW UPPER FACE	54.93015978	-0.0142105	Small inflow and outflow occurred across the lower boundary face.
FLOW BACK FACE	0	0	No flow occurred through the upper boundary.
Total Zone Flow	54.93015978	-0.0142105	Net outflow across the zone boundaries.
TOTAL FLOW	11,490.43	-11,490.43	Total inflow matches outflow, satisfying the mass balance principle.
Summary	In - Out	% difference	
Sources/Sinks	-54.91598322	-0.47907341	Summarizes flow due to sources and sinks, with no major discrepancies.

Cell To Cell	**54.91594928**	**199.8965463**	**Cell-to-cell flow is consistent with minimal difference, ensuring mass balance.**
Total	**-3.39388E-05**	**-2.95E-07**	**Extremely small differences validate that mass is conserved.**

Table 5.6: Layer 6 flow budget for transient simulated model

Interpretation:

- **Recharge** is the primary inflow into the system (4,758.55 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-simulated model.

5.2 TRANSIENT CALIBRATION FLOW BUDGET

5.2.1 Layer 1 flow budget

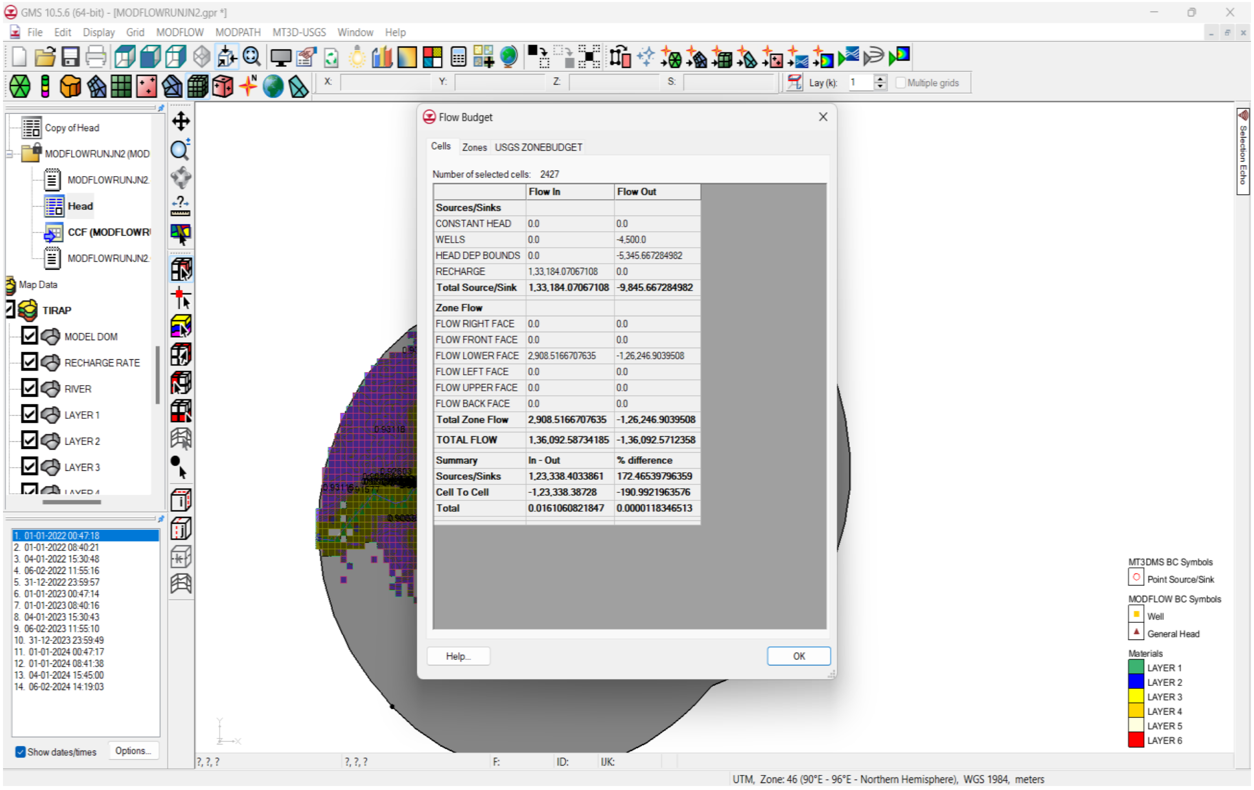


Fig 5.3 Layer 1 flow budget of calibrated model

Category	Component	Flow In	Flow Out	Description
Sources/Sinks	CONSTANT HEAD	0	0	No water exchange occurred at constant head boundaries.
	WELLS	0	-4,500.00	Wells extract 4,500 units of water, acting as a sink.
	HEAD DEP BOUNDS	0	-3,073.43	Outflow occurs to head-dependent boundaries.
	RECHARGE	96,232.61	0	Recharge is the primary inflow, adding significant water to the system.
	STORAGE	24,931.92	0	Additional water inflow due to storage effects.

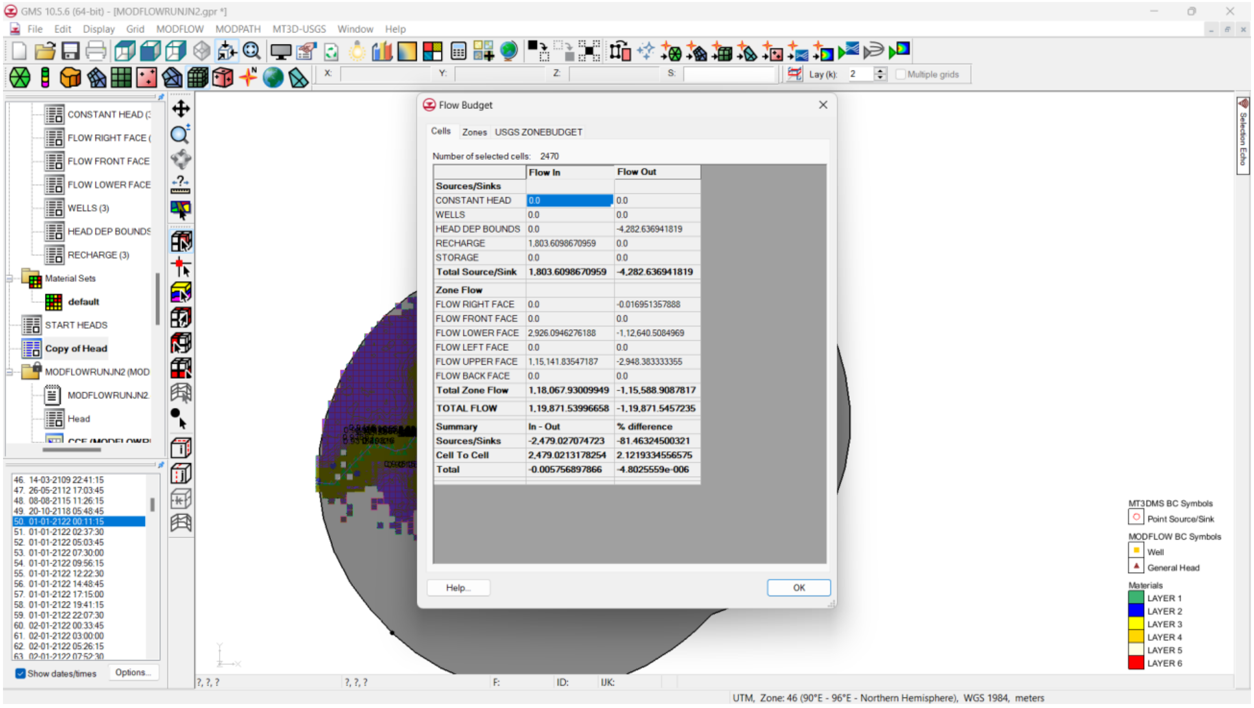
Table 5.7: Layer 1 flow budget for transient Calibrated model

	TOTAL Source/Sink	**1,21,164.52**	**-9,073.43**	**The net source/sink balance shows recharge and storage as major contributors.**
Zone Flow	**FLOW RIGHT FACE**	**0**	**-0.0007**	**Negligible flow across the right boundary.**
	FLOW FRONT FACE	**0**	**-0.0201**	**Minor outflow at the front boundary face.**
	FLOW LOWER FACE	**2,948.38**	**-1,15,039.43**	**Significant inflow and outflow through the lower boundary face.**
	FLOW LEFT FACE	**0**	**0**	**No flow occurred through the left boundary plane.**
	FLOW BACK FACE	**0**	**-0.0058**	**Negligible flow across the back boundary.**
	FLOW UPPER FACE	**0**	**0**	**No flow occurred through the upper boundary.**
	TOTAL Zone Flow	**2,948.38**	**-1,15,039.43**	**Net outflow is significant across the lower boundary face.**
TOTAL FLOW		**1,24,112.91**	**-1,24,112.89**	**The total inflow and outflow are nearly equal, ensuring mass conservation.**
Summary	**Sources/Sinks**	**1,12,091.08**	**172.13**	**Sources and sinks contribute the majority of inflow and minor outflow.**
	Cell-To-Cell Flow	**-1,12,091.08**	**190**	**Internal flows between cells are balanced.**

Interpretation: From the above table we can interpret that

- **Recharge** is the primary inflow into the system (96,232 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well calibrated model.

5.2.2 Layer 2



FLOW BUDGET TABLE FOR LAYER 2 (2022-2034)

Sources/Sinks Section:

This section summarizes the input/output of water from external sources or sinks in the model.

- **Flow In**: Water entering the model (inflow).
- **Flow Out**: Water leaving the model (outflow).

Term	Description	Value
Constant Head	Water entering or exiting through constant head boundary conditions. These boundaries maintain a fixed water level.	0.0 (no inflow or outflow)
Wells	Represents water extracted (negative) or injected (positive) through wells.	0.0
Head Dep Bounds	Water flow associated with head-dependent boundary conditions like rivers or drains.	0.0 In, -4222.6369 Out
Recharge	Recharge is water added to the system from precipitation or infiltration processes.	1803.6096
Storage	Represents changes in storage, typically caused by variations in hydraulic head over time (transient conditions).	0.0

Total Source/Sink	Sum of all inflow and outflow from the sources/sinks listed above.	1803.6096 In, -4222.6369 Out

Zone Flow Section:

This section accounts for water movement across model zone boundaries (faces).

- **Flow In**: Flow entering the zone through specific faces.
- **Flow Out**: Flow exiting the zone through specific faces.

Term	Description	Value
Flow Right Face	Water moving across the right boundary of a cell.	0.0 In, -0.0169 Out
Flow Front Face	Water moving across the front face of a cell.	0.0
Flow Lower Face	Flow through the lower face (bottom) of the cell.	2926.0946 In, -1126.6405 Out
Flow Left Face	Water entering/exiting the left boundary of a cell.	0.0
Flow Upper Face	Flow through the upper face (top) of the cell.	1151.1435 In, -2948.3333 Out
Flow Back Face	Represents flow through the back boundary of the cell.	0.0
Total Zone Flow	The net water movement across all zone boundaries (sum of all inflows and outflows across faces).	1180.679 In, -15588.9088 Out

Summary Section:

This section summarizes the total inflow, outflow, and their difference for all sources/sinks and cell-to-cell flow.

Term	Description	Value
Sources/Sinks	Total inflow and outflow from external sources/sinks (see "Sources/Sinks Section").	In: -2479.027 Out: -31.4623
Cell to Cell	Represents water movement within the model grid (internal flow between cells).	In: 2479.021 Out: 2.129
Total Flow	Overall total inflow and outflow within the system (combines sources/sinks and cell-to-cell flows).	In: -0.005 Out: -4.8025

% Difference:

- Represents the percentage difference between inflow and outflow, useful for checking mass balance errors.
- The values are very small (close to 0), indicating that the model is balanced.

Interpretation:

- **Recharge** is the primary inflow into the system (1803.6096 units).
- **Head Dependent Bounds** and **Zone Flow (Out)** contribute most of the outflow.
- The total inflow and outflow are nearly equal, with negligible mass balance errors, indicating a well-calibrated model.

5. CONCLUSION

This study demonstrated a conceptual model, built from subsurface exploratory data, incorporated aquifer properties, recharge conditions, and boundary constraints to simulate groundwater flow and contaminant transport under transient conditions. The simulations revealed that recharge is the primary inflow mechanism, while head-dependent boundaries and well extraction significantly contribute to outflows. Longitudinal dispersivity, transverse dispersivity, and molecular diffusion were identified as key factors influencing the spread of contaminants. The transient-state model accurately predicted the movement of ground water over a 100-year period, offering valuable data for groundwater management.

Despite some technical challenges, such as aborted MT3DMS runs due to source/sink limitations, the model achieved satisfactory calibration with minimal mass balance errors. This ensured reliable predictions of flow budgets across the aquifer layers and highlighted recharge zones as critical areas for contamination mitigation.

The study shows the importance of advanced groundwater modeling tools like MT3DMS in addressing environmental issues related to mining activities. Future research should incorporate reactive transport models to simulate chemical degradation processes, enhancing the predictive accuracy of contaminant fate and behaviour. Such advancements can support the development of targeted remediation strategies to safeguard groundwater resources in vulnerable regions like Tirap OCP.

Limitations:

1. **Modelling Complexity**: The heterogeneous and anisotropic nature of the Tirap aquifer system posed challenges in achieving a stable simulation. Accurate representation of subsurface properties required significant simplifications.
2. **Source/Sink Limitations**: MT3DMS runs were aborted due to exceeding source/sink limits in the input files, necessitating adjustments and re-runs with reduced complexity.
3. **Data Availability**: Limited field data on chemical reactions, groundwater extraction, and recharge rates required assumptions, potentially affecting model accuracy.
4. **Exclusion of Reactive Transport**: The study focused on physical transport processes (advection, dispersion) without incorporating reactive mechanisms like sorption or degradation, which are critical for contaminant dynamics.
5. **Temporal Constraints**: The long-term predictions (100 years) are subject to uncertainties in input parameters, particularly recharge and hydraulic conditions that may change over ti

6.REFERENCES

- Adeoye , Peter Aderemi; Jiya Musa John ,Kuti: Abayomi Ibrahim 2018 *Simulation of Heavy Metals Movement and Change in Concentration in Shallow Unconfined Aquifer in North Central Nigeria Using Visual Moflow and Mt3dms* **,** International Society of Waste Management of Air and Water , Vol 44 https://doi.org/10.5276/JSWTM.2018.51
- Anupam Chowdhury, Mumtahina Rahnuma 2023 *Groundwater contaminant transport modeling using MODFLOW and MT3DMS: a case study in Rajshahi City* Water Practice and Technology (2023) 18 (5): 1255–1272. https://doi.org/10.2166/wpt.2023.076
- Arlen W. Harbaugh, Edward R. Banta, Mary C. Hill and Michael G. McDonald. (2000). MODFLOW-2000, the U.S. Geological survey modular, groundwater model- user guide to modularization concepts and the groundwater flow process.
- Chunmiao Zheng, and P. Patrick Wang. (1999). MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection,Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems. http://www.geology.wisc.edu/~andy/g727/mt3dmanual.pdf.
- C.Zheng. (1990). A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems, pp.1-1
- Conceptual Model Approach and MT3DMS Tutorial by GMS AQUAVEO
- Gerald W. Recktenwald. (2011). Finite-Difference Approximations to the Heat Equation
- Jacob Bear , Alexander H.-D. Cheng,2010, Modeling Groundwater Flow and Contaminant Transport.
- P.Anil Kumar ,G.N Pradeep Kumar , M.J Nandan 2021 *Assessment of Contaminant migration using MT3DMS Model* , Conference Paper, Advanced Modelling and Innovations in Water Resources Engineering. Lecture Notes in Civil Engineering, vol 176. Springer, Singapore. https://doi.org/10.1007/978-981-16-4629-4_41
- Phoummixay Siharath[1], Somchay Vilaychaleun[2], Khampasith Thammathevo[3], Chankhachone Sonemanivong[4], Soulyphan Kannitha[5], Bounmy Phommakone[6], Keoduangchai Keokhamphui[7], Guillermo III Quesada Tabios[8] *Lead and Zinc Groundwater contaminant Transport Modelling Using MT3DMS In XAYSOMBOUN PROVINCE, LAO PDR*

  Asian Journal of Science, Technology, Engineering and art **https://doi.org/10.58578/AJSTEA.v1i2.1934**
- Sandip S. Sathe∗, Chandan Mahanta 2018 *Groundwater flow and arsenic contamination transport modeling for a multi aquifer terrain: Assessment and mitigation strategies*,Journal Of Environmental Management. https://doi.org/10.1016/j.jenvman.2018.08.057
- V.Pugazhendi Ground Water Modelling Report for Tirap OCP, North Eastern Coalfields, Tinsukia District, Assam State 2022 ,CMPDIL report .