NOVEL APPROACH TO GROUNDWATER CONTAMINANT TRANSPORT MODELLING

Manoj Kumar[1], Anunay Gour[2]

[1]Corresponding Author, Department of environmental engineering, Delhi Technological University, New Delhi, E-mail: m.kumar62.mk@gmail.com
[2]Department of environmental engineering, Delhi Technological University, New Delhi, E-mail: anunaygour@dtu.ac.in

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

Keywords: *groundwater, modelling, contaminant transportation, MODFLOW, FEFLOW, MT3DMS, RT3D, MODPATH*

1. Introduction

Groundwater modelling is a technique to understand a system's response under certain conditions or to anticipate the system's future behaviour by representing it in another form. Groundwater modelling is an effective tool for groundwater resources management and protection. A logical relation between the info availability and model complexity should be considered for better presentation. When there's a shortage of data, selecting complex systems wouldn't end in desirable results and wouldn't show the real scenario. In such situations, we should review our expectations of the model's ability as per the data availability and accessibility. Representation of the real-world problem in simple form without compromising the accuracy is a challenge for the modellers. To get the best description of the real world situations modellers tend to get the maximum data possible and the selection of the right model tool plays a vital role in the best representation of reality also. Classification of groundwater models can be done as a physical model, analogue model, and mathematical model. Physical models are the laboratory portrayal of the groundwater system such as the Sand tank which poses a scaling problem. Analogue models are the electronics models developed by the analogy between water flow systems and electrical flow systems (Delleur, 2006). For example, “Electrical current flow through a circuit board with resistors to represent hydraulic conductivity and capacitors as storage coefficient”. Representation of the groundwater system mathematically by a set of equations is known as a mathematical model. The mathematical models can be solved either numerically or analytically. Through the ages, analytical methods have become standard tools for explaining groundwater quantity and quality dynamics. Also, these models are occasionally applied before a numerical model starts. These models have their disadvantages concerning mathematical assumptions that may not occur naturally. Another problem is that they do not allow for simulating spatial and temporal variations in various parameters simultaneously. Hence, these models are often inadequate to mimic a heterogeneous subsurface system closely. “Numerical solutions can handle more complicated problems than analytical solutions. With the rapid development of computer processors and increasing speed, numerical modelling has become more effective and manageable”(Baalousha, 2005). A detailed explanation of numerical techniques is provided in the next chapter.

2. Numerical Models

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

2.1 Finite Difference Method

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

$$\frac{dy}{dx} = \lim_{\Delta x \to \infty} \left(\frac{\Delta y}{\Delta x} \approx \frac{\Delta y}{\Delta x} \right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots Eq.2.1$$

The finite difference method relies upon the calculation of a “function derivative by a finite-difference”. In this method, the area of concern is divided into small cells of regular shape or grid points called nodes, the derivatives of the partial differential equations are approximated in space, concerning the differences between values of variables at adjacent cells or nodes. The nodes represent the specific values of the system's computational properties (e.g., hydraulic head, solute concentration, effective porosity) as functions of time. All nodes are defined in a body-fitted coordinate system and labelled consecutively by a set of indices (i, j, and k along the direction x, y, and z respectively). Discretization of the area in the finite difference method within a model domain is presented in figure 2.1. FDM is well documented easy to implement and gives reasonably good results. The main limitation of the finite difference method is that we can not apply it appropriately to the irregular shape boundaries as the area of concern is divided into regular shape cells. Accuracy and the efforts required for computation are positively affected by the grid size and their distribution. “The output accuracy of the finite difference method is useful in the case of solute transport modelling. Mass balance is not guaranteed if conductivity or grid spacing varies”(Baalousha, 2005).

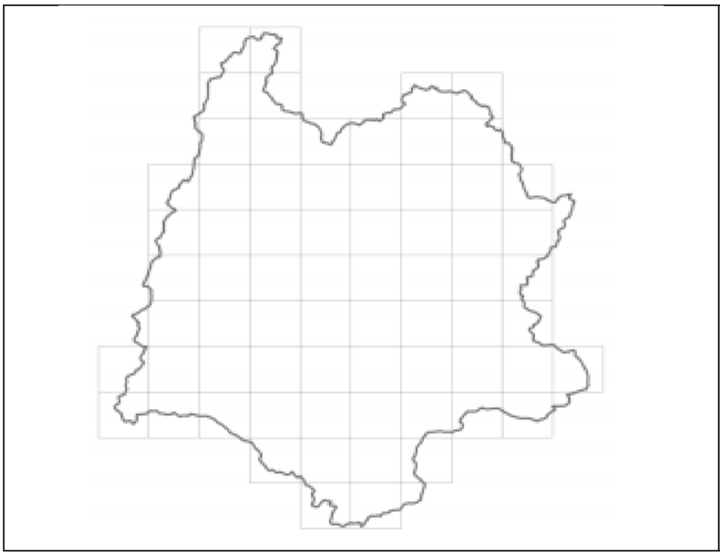

Fig2.1 Discretization of space in FDM(Elango, 2005)

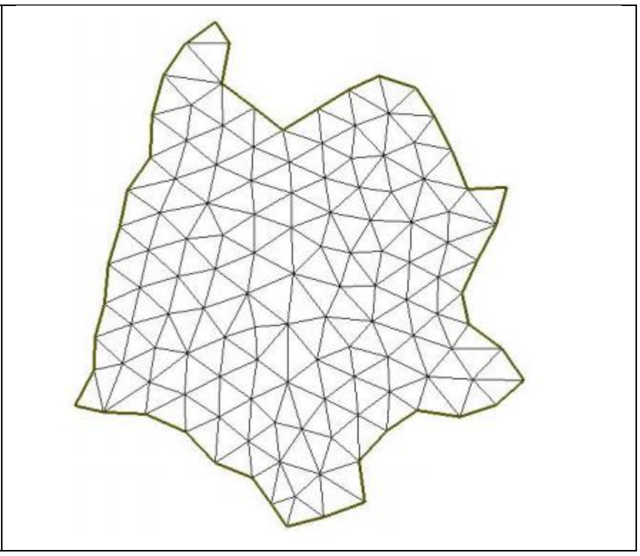

Fig 2.2 Discretization of space in FEM

2.2 Finite element method

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

3. Modelling approach

Identification of model objectives is the first step in any modelling. A critical concern in the modelling process is data collection and processing. However, model conceptualization is the most fundamental step in modelling. After completion of the model and the first run, calibration, verification, and sensitivity analysis can be performed. The steps involved in groundwater modelling are shown in Figure 3.1.

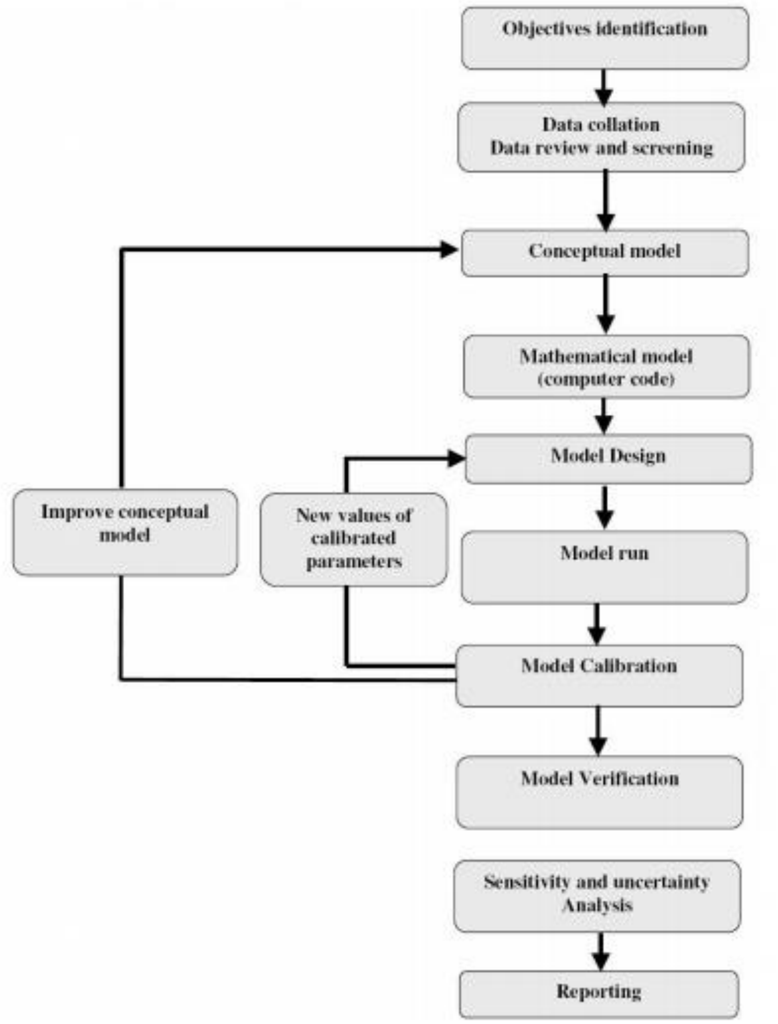

Fig 3.1 Modelling process flow chart(Baalousha, 2005).

3.1. Formulating modelling objectives

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

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

3.2 Conceptual Model

Model conceptualization is a qualitative description of a ground-water system that includes the information of the water balance, hydrological and geological conditions. Model conceptualization is the most important part of groundwater modelling. After the identification of model objectives, it is the next step in the model development. Data about Geology, hydrology, boundary conditions and hydraulic parameters are needed to

develop a conceptual model. A good conceptual model must be able to represent real-world situations in a simple manner that meets modelling goals and management requirements. In the case of groundwater quality modelling, it must outline our interpretation of contaminant transport or water flow.
The key factors that the conceptual model should contain are:

1. Model domain area
2. Aquifer’s geometry
3. Sources and sinks identification
4. Groundwater recharge
5. Boundary conditions
6. Aquifer properties like Porosity, Hydraulic conductivity, Storativity
7. Water balance

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

3.2.1. Boundary Value Problem

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

$$\frac{d^2h}{dx^2} + \frac{d^2h}{dy^2} + \frac{d^2h}{dz^2} = 0 \text{..eq. (3.1)}$$

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

3.2.2. Boundary Conditions

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

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

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

3.3. Selection of modelling software

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

3.4. Model Design

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

3.5. Model Calibration

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

3.6. Model Verification

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

3.7. Sensitivity Analysis

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

3.8. Uncertainty Analysis

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

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

4. Migration of Solutes in Groundwater

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

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

4.1. Governing Equations

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

$$\frac{\partial}{\partial x}\left(wD_{xx}\frac{\partial c}{\partial x}+wD_{xy}\frac{\partial c}{\partial y}+wD_{xz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial y}(wD_{yy}\frac{\partial c}{\partial y}+wD_{yx}\frac{\partial c}{\partial x}+wD_{yz}\frac{\partial c}{\partial z})+\frac{\partial}{\partial z}\left(wD_{zz}\frac{\partial c}{\partial z}+wD_{zy}\frac{\partial c}{\partial y}+wD_{zx}\frac{\partial c}{\partial x}\right)-\left(q_x\frac{\partial c}{\partial x}+q_y\frac{\partial c}{\partial y}+q_z\frac{\partial c}{\partial z}\right)=\rho_b\frac{\partial s}{\partial t}+\frac{\partial wc}{\partial t}+K_m wC^m\pm R \text{.........eq. (4.1)}$$

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

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

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

$$\mathrm{R} = 1+\frac{\rho_b}{n}K_d \text{.........eq. (4.2)}$$

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

$$D_{xx} = \varepsilon_L\frac{v_x^2}{v}+\varepsilon_T\frac{v_y^2}{v}+\varepsilon_T\frac{v_z^2}{v}+D^* \text{.........eq. (4.3)}$$

$$D_{yy} = \varepsilon_L \frac{v_y^2}{v} + \varepsilon_T \frac{v_x^2}{v} + \varepsilon_T \frac{v_z^2}{v} + D^* \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.4)}$$

$$D_{zz} = \varepsilon_L \frac{v_z^2}{v} + \varepsilon_T \frac{v_x^2}{v} + \varepsilon_T \frac{v_y^2}{v} + D^* \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.5)}$$

$$D_{xy} = D_{yx} = (\varepsilon_L - \varepsilon_T)\frac{v_x v_y}{v} \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.6)}$$

$$D_{xz} = D_{zx} = (\varepsilon_L - \varepsilon_T)\frac{v_x v_z}{v} \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.7)}$$

$$D_{yz} = D_{zy} = (\varepsilon_L - \varepsilon_T)\frac{v_z v_y}{v} \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.8)}$$

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

$$\frac{\partial}{\partial x}(K_{xx}\frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - Q = S_s\frac{\partial h}{\partial t} \ldots\ldots\ldots \text{eq. (4.9)}$$

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

$$Q = \sum_{i=1}^{r} Q_i\, S(x - x_i)(y - y_i)(z - z_i) \ldots\ldots\ldots\ldots\ldots\ldots \text{eq. (4.10)}$$

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

5. Simulator software for transport and groundwater flow modelling

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

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

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

Visual MODFLOW is one of the user-friendly and most important simulation environments to simulate three-dimensional contaminant transport and groundwater flow. The software's instructions were simple, and it could only simulate groundwater flow below the water table, according to the instructions. MODFLOWSURFACT, MODFLOW, ZoneBudget, MODPATH, MGO WinPEST and MT3D/RT3D, are all included in the Visual MODFLOW software kit with graphical user interface (Fouad et al., 2018).

The MT3DMS is a three-dimensional numerical model that can be used to simulate solute transport in complicated hydrogeologic settings. It is MODFLOW's 3-D advection, dispersion, sorption, and reaction simulation module. It can be used in both saturated and unsaturated areas. MT3DMS can also simulate heat transfer in the presence of minor buoyancy and viscosity changes. In MT3DMS, chemical reactions such as advection-dispersion and diffusion are involved. It was created using the Finite Difference Method by (Chunmiao Zheng, 1990). Specifically designed to manage “advectively-dominated transport problems without the need to construct refined models for solute transport”.

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

II. FEFLOW (finite element subsurface and transport system)

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

It is capable of computing:

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

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

The workflow of FEFLOW and MODFLOW based on the conceptual model is shown in figure 5.1.

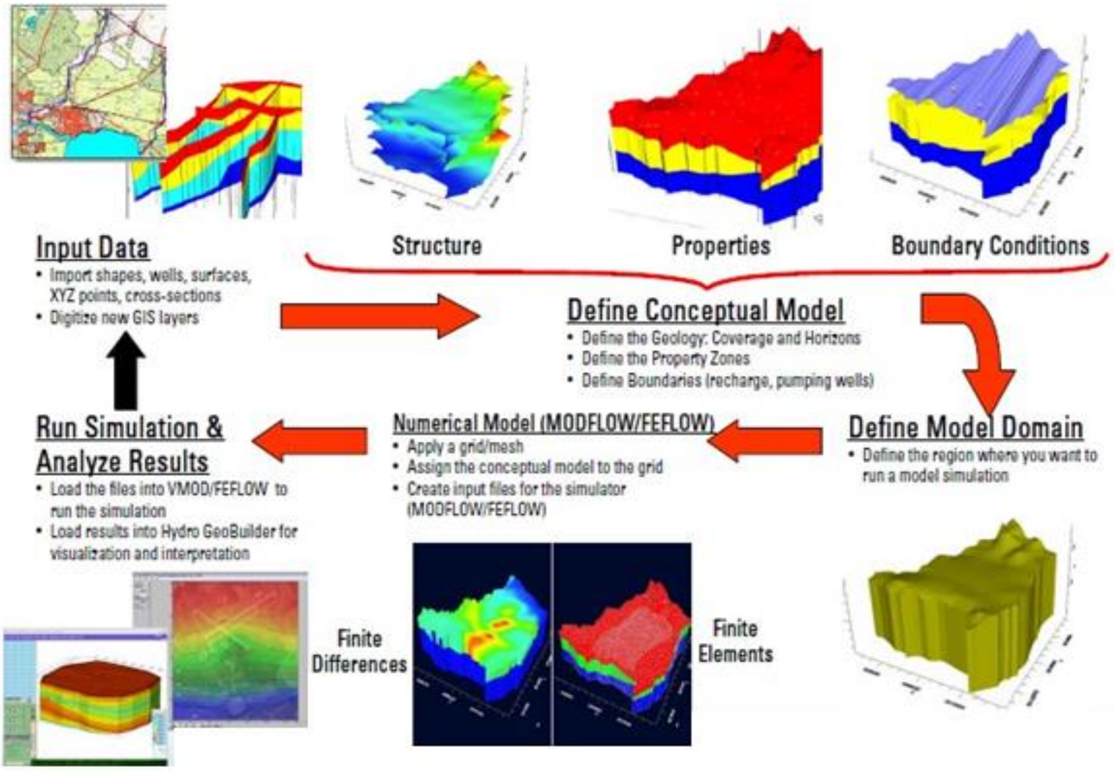

Fig 5.1 Workflow of FEFLOW and MODFLOW(Fouad et al., 2018)

III. HST3D (3-D Heat and Solute Transport Model)

HST3D (Heat and Solute Transport Model) is used to simulate groundwater flow and related heat and solute transport in 3D form. It is an effective and user-friendly interface built into the Argus ONE (Argus Open Numerical Environments) modelling environment. Users can input all spatial data, run HST3D graphically, and visualize the output using HST3D. Within one comprehensive graphical user interface (GUI) Argus ONE incorporates GIS, CAD, Database, Geostatistics, Conceptual Modelling, Automated Grid and Mesh Creation, and Scientific Visualization(Kipp, 1997). The HST3D model can be used to examine issues such as – freshwater recharge and recovery, contaminant plume movement, subsurface waste injection, landfill leaching, geothermal water systems, hazardous waste disposal, the intrusion of saltwater, subsurface energy storage and other transportation-related issues (Kumar, 2012). To run HST3D, you'll need the Argus ONE GIS and Grid Modules. Only the heat- or solute-transport equation is solved in combination with the ground-water flow in most applications.

IV. SUTRA(3-D Saturated/Unsaturated Transport Model)

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

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

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

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

V. Use of GIS and Meshfree techniques

With the aid of various geo analysts and spatial statistical methods, a large number of GIS-based systems have been used in recent years to classify regions vulnerable to contamination(Shrimali et.al,. 2019). ArcGIS Model Builder and Visual Basics (VB) software can be used to develop a GIS-based Contaminant Transport Model (GIS-CONTRAM) to demonstrate the fate of contaminants transport in the subsurface (Menezes, 2009). When checked with Visual MODFLOW, the CONTRAM model achieved fair results. The element free Galerkin method (EFGM) is a sufficiently accurate and simple method for numerically simulating contaminant transport in two dimensions through saturated homogeneous porous media and landfill liners. In the EFGM, an estimated solution is designed entirely in terms of a series of nodes, and no characterization of the nodes interrelationship is needed. The EFGM approximates the function with moving least square approximants and imposes critical boundary conditions with the Lagrange multiplier process. The EFGM findings and the data from the field investigation are in good agreement(Praveen Kumar & Dodagoudar, 2009).

6. CONCLUSION

This study indicates that the knowledge of the basics of groundwater modelling, selection of the right numerical or analytical model and clear model objective will solve any problem related to contaminant transport in groundwater. The selection of appropriate models is governed by factors such as aquifer properties, hydrogeology, type of pollutants, and the solute transport process that occurs in one's study area. Model calibration is also an important step in model development and it can be done manually or automatically. The finite difference method is used by MODFLOW-based software, while the finite element method is used by software like FEFLOW. No method is ideal, and each method has its own set of advantages and drawbacks. For numerically simulating contaminant transport in two dimensions, the mesh-free design is a sufficiently accurate and simple process. The outcomes of the EFGM and the evidence from the field investigation are quite similar. New methodologies, such as Arc Hydro Groundwater executable programming code and GIS CONTRAM, can be built by merging GIS and GMS.

REFERENCES

Baalousha, H. (2009). Fundamentals of groundwater modelling. *Groundwater: Modelling, Management and Contamination; Konig, LF, Weiss, JL, Eds*, 149-166.

Baalousha, H., & Köngeter, J. (2006). Stochastic modelling and risk analysis of groundwater pollution using FORM coupled with automatic differentiation. *Advances in Water Resources*, *29*(12), 1815–1832. https://doi.org/10.1016/j.advwatres.2006.01.006

Clement, T. (1997). A Modular Computer Code for Simulating Reactive Multi-Species Transport in 3-D Groundwater Systems. PNNL-11720. *Pacific Northwest National Laboratory, Richland, WA. 59 pp.*

Shrimali N. J, Daksh H Soni, M. A. M. (2019). *A Study of Various Approaches for Groundwater Contaminant*. http://iwwa-ahmedabad.org/images/downloads/papers/2019/1913.pdf

Elango, L. (2005). Numerical Simulation of Groundwater Flow and Solute Transport. *Allied Publishers Pvt. Ltd.pp.151-164. January 2005.*

FEFLOW 7.3 Documentation - Introduction. (n.d.). Retrieved June 30, 2021, from http://www.feflow.info/html/help73/feflow/01_Introduction/intro.htm

Fouad, M., Hussein, E. E., & Jirka, B. (2018). Assessment of Numerical Groundwater Models. *International Journal of Scientific & Engineering Research*, *9*(6), 951–974. http://www.ijser.org

Harbaugh, A. W. (2005). The U.S. Geological Survey Modular Ground-Water Model — the Ground-Water Flow Process. *U.S. Geological Survey Techniques and Methods 6-A16*, 253.

Kipp, K. L. (1997). Guide to the revised heat and solute transport simulator: HST3D- Version 2. *U.S. Geological Survey Water-Resources Investigations*, *97–4157*, 1–158.

Koukidou, I., & Panagopoulos, A. (2010). Application Of FEFLOW For The Simulation Of Groundwater Flow At The Tirnavos (Central Greece). *Bulletin of the Geological Society of Greece*, *43*(2010), 1747–1757.

Kumar, C. P. (2003). Introduction to Groundwater Modelling. (Vol. 247667). http://nihroorkee.gov.in/sites/default/files/uploadfiles/CPK_GW_Modelling.pdf

Kumar, C. P. (2012). Groundwater Modelling Software – Capabilities and Limitations. *IOSR Journal of Environmental Science, Toxicology and Food Technology*, *1*(2), 46–57. https://doi.org/10.9790/2402-0124657

Pinder G., G. W. (1978). Finite element simulation in surface and subsurface hydrology. *Advances in Water Resources*, *1*(3), 175. https://doi.org/10.1016/0309-1708(78)90029-5

Praveen Kumar, R., & Dodagoudar, G. R. (2009). Modelling of contaminant transport through landfill liners using EFGM. *International Journal for Numerical and Analytical Methods in Geomechanics*, *34*(7), n/a-n/a. https://doi.org/10.1002/nag.817

Summary of SUTRA. (n.d.). Retrieved March 11, 2021, from https://water.usgs.gov/cgi-bin/man_wrdapp?sutra(1)

Wang, D., Wu, C., Huang, W., & Zhang, Y. (2019). Vibration investigation on fluid-structure interaction of AP1000 shield building subjected to multi earthquake excitations. *Annals of Nuclear Energy*, *126*, 312–329. https://doi.org/10.1016/j.anucene.2018.11.021

Zheng, C., & Wang, P. (1998). MT3DMS: A modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems. *US Army Corps of Engineers Engineer Research and Development Center*, *June*, 239. http://www.geo.tu-freiberg.de/hydro/vorl_portal/gw-modellierung/MT3DMS Ref Manual.pdf