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Numerical Modelling of Two Dimension Contaminant Transport Equation in Riverbank System

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Abstract
The contamination of riverbanks has become a major environmental concern in recent years. A natural method of treating river water is riverbank filtration (RBF) technology. Water from the river began to flow towards the pumping well, which was next to the river, as a result of the pumping operation. Due to the chemical, physical, and biological processes that took place in the riverbed sediments, the contaminants are eliminated from the water as it travels from the river to the pumping well. We developed a two-dimensional contaminant transport model to simulate the movement of contaminants in a riverbank filtration system. The model takes into account the velocity and dispersion of water, as well as the adsorption and decay of contaminants. The two-dimension contaminant transport equation is a mathematical model used to simulate the movement of pollutants in two-dimensional spaces, such as bodies of water or underground aquifers. This equation takes into account the physical processes of advection, diffusion, and dispersion to predict the concentration of contaminants at different points in time and space. Hence, finite difference method (FDM) is use to solve the equation. Thus, steady-state head distribution in the first model layer and the steady-state hydraulic head distribution in the third model layer and capture zones of pumping wells captured.

Keywords: Riverbank filtration; two-dimension contaminant transport; finite difference method

1. Introduction

Riverbank filtration (RBF) technology is a natural method of treating river water. Contaminants in the water are eliminated as it flows from the river to the pumping well due to chemical, physical, and biological processes in the riverbed sediments. Hydraulic conductivity, which represents the fluid's ability to travel through porous materials, is a crucial factor in estimating pollutant travel time. The hydraulic conductivity varies significantly depending on the soil type. Aquifer pumping tests are commonly used to determine hydraulic conductivity, but in their absence, approximations based on grain size or published values are used. Numerical solutions are required for complex cases where analytical models are not applicable. This research aims to study the effect of hydraulic conductivity on pollutant transport in riverbank filtration systems using the finite difference method. The research also investigates the impact of the distance between the contamination source and the pumping well. Surface water contamination is primarily caused by human activities, posing risks to both humans and wildlife. Riverbank filtration is an effective technique for treating contaminated surface water. However, there is a need to develop a model to simulate contamination behavior in such systems. Understanding contaminant behavior and the parameters influencing their transit in groundwater systems is crucial for effective planning and management of riverbank filtration systems.

Contaminant concentration is a critical aspect that affects groundwater quality. The increase in contaminant concentration in pumped water is mainly due to the groundwater influx, which is influenced by hydraulic conductivity. Mathematical modeling is necessary to estimate the influence of hydraulic conductivity on pollution movement. This research focuses on the numerical modeling of two-dimensional contaminant transport in riverbank filtration systems using the finite difference method. Specifically, it considers chemical contaminants present unintentionally in food or feed. The research utilizes the MODFLOW software for implementing the finite difference method. Contaminated surface water poses significant health risks to humans and wildlife. The proposed model for simulating contaminant transport in riverbank filtration systems can contribute to the effective management and mitigation of surface water contamination. By using the model, valuable time and resources can be saved. Additionally, the model can be applied by companies and engineers to predict and forecast the spread of contaminants near pumping wells, considering the effects of pumping processes and hydraulic conductivity parameters.

2. Research Methodology

In this study, the Finite Difference Method is utilized to solve groundwater flow equations and obtain important parameters such as flow rates, flow direction, and hydraulic heads in an aquifer. The research aims to provide a comprehensive understanding of the Finite Difference Method and its application in groundwater modeling. The MODFLOW software is one example of a programming tool that implements the finite difference method for solving groundwater flow equations. The grid used in the finite difference method consists of discrete, rectilinear (rectangular) cells. This approach is widely accepted and employed by various regulatory bodies. MODFLOW, being an open-source and well-documented software, is widely used as a groundwater simulator. The finite difference method offers simplicity in understanding and calculating solutions, while ensuring mass conservation. Moreover, it provides various numerical extensions such as PEST, transport, particle tracking, and zone budget analysis. However, the finite difference method has certain limitations. The grid design, although straightforward, may not allow efficient adjustments around specific points of interest like wells and model boundaries. To address this issue, the MODFLOW-LGR (Local Grid Refinement) modification can be employed, which partially resolves the limitations of the traditional finite difference approach.

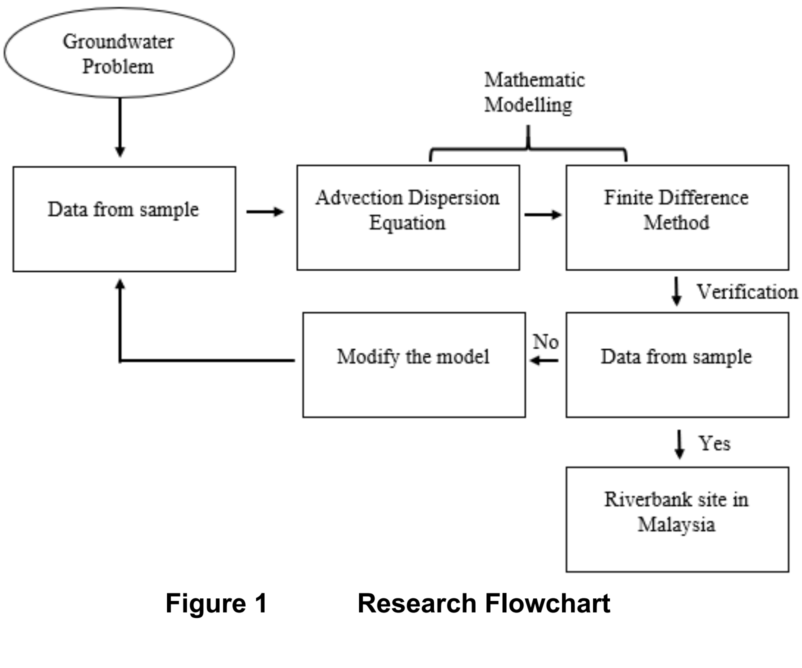

Figure 1 Research Flowchart

3. Advection Dispersion Equation

The advection dispersion reaction (ADR) equation is used to describe solute transport in various groundwater transport models. The ADR equation, as shown below, represents the change in dissolved solute concentration (C) over time (t) when groundwater flow is oriented in the x direction.

$$\frac{dc}{dt} = Dx\frac{d^2c}{dx^2} + Dy\frac{d^2c}{dy^2} - v\frac{dc}{dx} - \lambda Rc$$

The rate of mass change per unit volume is the term on the left side of the equation. On the right, terms reflect solute flux due to dispersion in the x and y directions, advective flux in the x direction, and first order decay due to biotic and abiotic processes. The following relationships are typically used to estimate dispersion coefficients (Dx/Dy):

$$D_x = D_m + v\alpha_L$$

$$D_y = D_m + v\alpha_T$$

3.1 Finite Different Method

The finite difference method (FDM) is a method for solving partial differential equations that is approximate. Linear and nonlinear issues, as well as time independent and dependent problems, are examples of these. This method can be used to solve problems with a range of border forms, boundary conditions, and a region made up of a variety of materials. The basic idea is to use approximation derivation formulae to substitute the derivatives in the (ordinary or partial) differential equation and the starting or (and) boundary conditions, resulting in a "approximating system of equations" to solve the function. The most general linear equation for second order differential equation can be written as:

$$y"(x) + p(x)y'(x) + q(x)y(x) = r(x), \qquad a \le x \le b$$

Specify the value of the solution at two points (boundary conditions):

$$y(a) = A \quad \text{and} \quad y(b) = B$$

Divide the interval I = [a, b] into n of subintervals of equal size. Thus, step size can be estimate by using:

$$h = \frac{b-a}{n}$$

First derivative, forward FD:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

First derivative, backward FD:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

First derivative, central FD:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Second derivative, central FD:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

$y_1, y_2, \dots, y_{n-1}$ can be calculated at any mesh point $x = x_i$, the finite-difference representation of the differential equation can be written as follows (based on central FD)

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + p_i\frac{y_{i+1} - y_{i-1}}{2h} + q_i y_i = r_i, \qquad (i = 1,2, \dots, n-1)$$

$$2(y_{i+1} - 2y_i + y_{i-1)} + hp_i(y_{i+1} - y_{i-1}) + 2h^2 q_i y_i = 2h^2 r_i, \qquad (i = 1,2, \dots, n-1)$$

and arranging the equations with respect to $y_1, \dots, y_n$, we can obtain the system of linear equations:

$$(2 + hp_i)y_{i+1} + (2h^2q_i - 4)y_i + (2 - hp_i)y_{i-1} = 2h^2r_i, \qquad (i = 1,2,\dots,n-1)$$

The boundary conditions provide of the solution at the two ends of the grid: $y_0 = A$ and $y_n = B$. We can interpret y as a vector and write the equation formally as an algebraic matrix equation:

$$A_hY_h = R_h$$

where

$$A_h = \begin{bmatrix} (2h^2q_1-4) & (2+hp_1) & 0 & \cdots & \cdots & 0 \\ (2-hp_2) & (2h^2q_2-4) & (2+hp_3) & 0 & \cdots & 0 \\ 0 & (2-hp_3) & (2h^2q_3-4) & (2+hp_3) & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & (2-hp_{n-2}) & (2h^2q_{n-2}-4) & (2+hp_{n-2}) \\ 0 & \cdots & \cdots & 0 & (2-hp_{n-1}) & (2h^2q_{n-1}-4) \end{bmatrix},$$

$$R_h = \begin{bmatrix} 2h^2r_1 - (2-hp_i)A \\ 2h^2r_2 \\ 2h^2r_3 \\ \vdots \\ 2h^2r_{n-1} \\ 2h^2r_{n-1} - (2+hp_{n-1})B \end{bmatrix}$$

$$Y_h = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-2} \\ y_{n-1} \end{bmatrix}$$

3.2 Mathematical Formulation

The suggested model was created to simulate pollutant movement to a pumping well placed L(L) distance from the river (Figure 2)

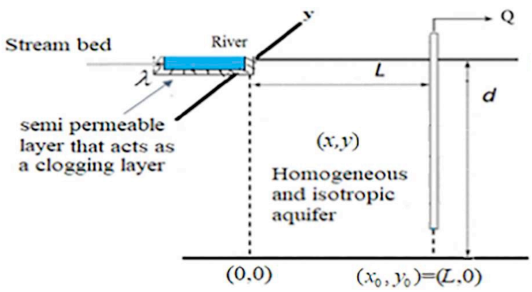

Figure 2 Conceptual model of the river bank filtration system

Based on the two assumptions that we are considering which are the domain's left and right boundaries have fixed hydraulic head values and the domain's north and south boundaries have no flow boundary conditions the flow can be considered uniform along the x-direction. (Libera et al., 2017). By letting the pumping rate Q(L3/T) is constant and the aquifer is homogeneous, isotropic, and has a finite depth d. (L).

$$\frac{R\partial C}{\partial t} = D_x\frac{\partial^2}{\partial x^2} + D_y\frac{\partial^2}{\partial y^2} - U_x\frac{\partial C}{\partial x} - vRC, \tag{1}$$

which gives the following equation:

$$\frac{R\partial C}{\partial t} - D_x \frac{\partial^2}{\partial x^2} - D_y \frac{\partial^2}{\partial y^2} + U_x \frac{\partial C}{\partial x} + vRC = 0, \quad (2)$$

where C(x,y,t) is the contaminant concentration (M/L^3); D_x, D_y are the components of the longitudinal and transverse dispersion coefficients along the x and y axes, respectively (L^2/T); U_x is the seepage velocity (L/T); v is the decay constant (1/T); R is the linear retardation factor; $Dx = a_l U_x$& $D_y = a_t U_x$ (Batu, 2005) are the dispersion coefficient If the equation β= vR is substituted, the equation becomes:

$$\frac{R\partial C}{\partial t} - D_x \frac{\partial^2}{\partial x^2} - D_y \frac{\partial^2}{\partial y^2} + U_x \frac{\partial C}{\partial x} + \beta C = 0, \quad (3)$$

where β is degradation rate of contaminant at (1/T). C_{in}(x,y,t) and G_{ads}(x,y,t) were utilised to indicate the concentration of contaminant penetration inside the aquifer and the concentration attenuated by bacteria, respectively. Using a balanced equation, we get:

$$C_{in} - C_{ads} = C_w \quad (4)$$

where C_w(t) is the value of the contaminant concentration in the pumping well water ($M/(L^3.T)$). It is not required that C_w(t) be zero. If C_w(t) = 0, the water can be made accessible to the public as drinking water right away. If, on the other hand, C_w(t) does not equal zero, which is more likely, then extra treatment can be performed prior to distribution. The degree of filtering and the concentration of pollutants in the pumped water determine this phase. As a result, Equation (3) is adjusted as follows:

$$\frac{R\partial C}{\partial t} - D_x \frac{\partial^2}{\partial x^2} - D_y \frac{\partial^2}{\partial y^2} + U_x \frac{\partial C}{\partial x} + \beta C = -C_w(t)\vartheta(x - x_0)\vartheta(y - y_0), \quad (5)$$

with the following initial and boundary conditions:

$$C(x, y, t) = 0x \to \infty,\ -\infty \le y \le \infty\ and\ t \ge 0 \quad (6)$$

$$C(x, y, t) = 0y \to \pm\infty,\ -\infty \le x \le \infty\ and\ t\ \ge 0 \quad (7)$$

$$C(x, y, t) = S_0 f(t, y)x = 0,\ -M \le y \le M\ and\ t\ \ge 0 \quad (8)$$

$$C(x, y, 0) = 0,\ \ 0 < x < \infty,\ -\infty \le y \le \infty\ and\ t\ \ge 0 \quad (9)$$

where β is the dimensionless Dirac delta function. M is the length of the river affected by the pumping well, S0($M/(L^3.T)$) denotes the starting mass of contaminants dissolved in one unit volume of water in one unit of time, and f(t,y) denotes a function of t and y, indicating that the river is not a uniform source of contaminants. Assume that adsorption with a linear isotherm reduces the concentration of contaminants released into the river. As a result, the function Cw (t) from Equation (4) can be computed as follows (Dillon et al., 2002):

$$C_w(t) = q/QS_0 \exp\left(-\frac{\beta t}{R}\right) \quad (10)$$

4. Result and Discussion

So, the following solution can be obtained:

$$C_D = -1/\left(4R\sqrt{\pi}\right)qQ \int_0^{t_D} 1/\sqrt{\tau_D} \exp\left(-(x_D - L_D)^2/(4 - \tau_D)\right)\left(erfc\left(\frac{y_D + M_D}{2\sqrt{\tau_D}}\right)\right) - \left(erfc\left(\frac{y_D - M_D}{2\sqrt{\tau_D}}\right)\right)) d_{\tau D}$$

(11)

Which becomes:

$$C(x,y,t) = S_0/(4R\sqrt{\pi})q/Q\sqrt{\frac{d}{U_x}}\exp\left(-\frac{\beta t}{R}\right)\int_0^t \frac{1}{\sqrt{\tau}}\exp\left(\frac{-\sqrt{R}(1/D_x(x-L-U_x\tau/R)^2}{4\tau}\right)$$
$$(erfc((\sqrt{R}(y+M)))/(2\sqrt{D_y t_y})) - erfc(((\sqrt{R}(y-M)))/(2\sqrt{D_y t_y})))d_\tau \qquad (12)$$

In the case of 1D groundwater flow (y = 0), the 1D Green's function will be used. Hence, Equation (12) will be converted to:

$$C(x,t) = 1/(2\sqrt{\pi}R)q/QS_0\sqrt{\frac{d}{U_x}}\exp\left(-\frac{\beta t}{R}\right)\int_0^t \frac{1}{\sqrt{\tau}}\exp\left(-R\left(x-\frac{U_x}{R}\tau^2/(4D_x\tau\right)d\tau\right. \qquad (13)$$

which leads to

$$C(x,t) = \frac{\frac{1}{(2\sqrt{\pi R})q}}{QS_0\sqrt{\frac{d}{U_x}}}\exp\left(-\frac{\beta t}{R}\right)\left(2\sqrt{\frac{U_x t}{d}}\exp\left(-\frac{R\left(x-\frac{U_x t}{R}\right)^2}{4D_x t}\right)\right) - \sqrt{\frac{\Pi R}{a_1 d}}\left(x-\frac{U_x t}{R}\right) erfc\left(\frac{\sqrt{R}\left(x-\frac{U_x t}{R}\right)}{2\sqrt{D_x t}}\right) \qquad (14)$$

MODFLOW OUTPUT

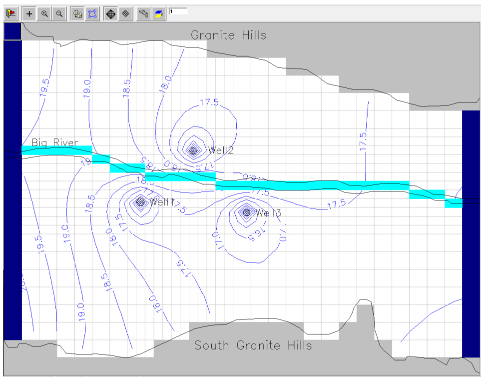

Figure 3: Steady-state head distribution in the first model layer

The steady-state head distribution in the first model layer of MODFLOW represents the spatial distribution of hydraulic head values under steady-state conditions (Figure 3). It is obtained through iterative numerical simulations that consider the groundwater flow equations, boundary conditions, and aquifer properties. This distribution provides valuable insights into groundwater behaviour and helps in making informed decisions regarding water resources management. Figure 4 shows the head of contour maps. The smallest head values on the map, or the lowest contours, typically indicate areas near pumping wells where the drawdown is the greatest. These maps provide valuable insights into groundwater flow patterns, well influence zones, and can aid in groundwater management and decision-making processes. When analysing a contour map of hydraulic heads, the contour lines connect points of equal head values. Typically, contour lines form closed loops, with higher head values in the centre of the loop and progressively lower values towards the outer parts. The contour interval, or the difference in head values between adjacent contour lines, is typically specified in the map. Regarding the statement that the smallest head on a contour map indicates proximity to a pumping well, this is generally correct in pumping scenarios. When a well is actively extracting groundwater from an aquifer, it creates a cone of depression around the well. The cone of depression represents an area of lower hydraulic head values caused by the pumping-induced drawdown. After performing steady-state flow simulation, extract and view result by using PMPATH. To delineate the capture zones of the pumping wells. Add New Particles dialog box appears, edit Particles on circles such that the number of particles is equal to 15, the radius R = 80 and the number of planes NK=3. Change the colour of new particles to Blue. Repeat the step by using Well 2 and Well 3 by using different colour. Set Exaggeration=25, Projection Row=15 and Projection Column=9. In the Tracking Steps group, change the (time) unit to years, step length to 10 and maximum number of steps to 200 and run the code.

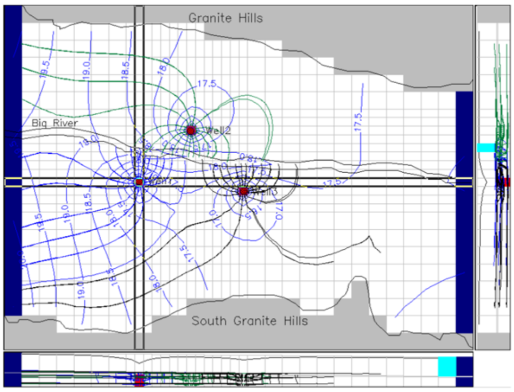

Figure 4: Steady-state hydraulic head distribution in the third model layer and capture zones of pumping wells

In groundwater modelling, the steady-state hydraulic head distribution refers to the spatial pattern of hydraulic head values in a specific layer of an aquifer system under steady-state conditions. The third model layer refers to the particular layer of interest in the model, which could be deeper or shallower depending on the specific modelling setup (Figure 4). When pumping wells are present in an aquifer system, they create a cone of depression in the groundwater table or piezometric surface. The cone of depression represents a localized area where the hydraulic head values are lower due to the pumping-induced drawdown. The capture zone of a pumping well refers to the area from which groundwater is drawn into the well. It represents the extent of influence or the region of the aquifer that contributes water to the well. The boundaries of the capture zone are defined by hydraulic gradients and the distribution of hydraulic head values. Thus, the capture zones of pumping wells can be identified by analysing the flow paths and hydraulic gradients, which are influenced by the distribution of hydraulic head values. These analyses help in understanding the behaviour of groundwater and making informed decisions regarding well placement and groundwater resource management. To run forward particle tracking, introduce a contaminant source upstream of Well 2 and see how far the contamination moves through the steady state flow field after 75, 100 and 125 years. Add New Particles dialog box you will notice that the figure defines the various faces of an individual cell, since the contamination is a surface source, we only want to place particles on cell face 5. Set the number of particles on Face 5 to NI=4 and NJ=4 and set NI and NJ on all the other faces to 0. In the Tracking Steps group, change the (time) unit to years, step length to 1, and maximum number of steps to 75. When finished, click OK to leave the dialog box.

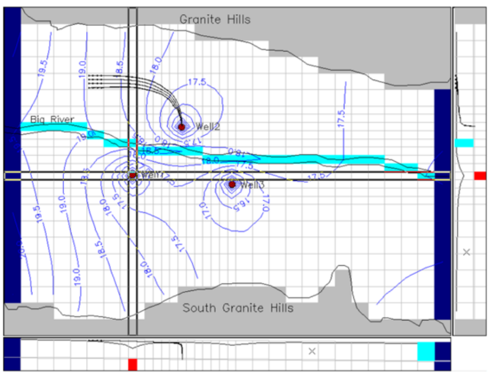

Figure 5: 125 years streamlines; particles are started at the cell [6, 5, 1] and flow towards Well 2

The concept of streamlines is used to analyse the flow of groundwater over an extended period of 125 years (Figure 5). Streamlines represent the paths that water particles would follow if they were released into the groundwater system. These streamlines provide valuable insights into the direction and patterns of groundwater flow. Well 2 is present is a pumping well present in the aquifer system. To determine the streamlines over a 125-year period, groundwater modelling software or numerical methods are typically employed. These methods utilize the hydraulic conductivity and hydraulic head distribution within the aquifer to simulate groundwater flow and particle movement.

Starting at cell [6, 5, 1], which represents a specific location in the model, the modelling software would trace the paths of water particles backward in time towards Well 2. The direction of the streamlines is influenced by the hydraulic gradients, which are determined by the distribution of hydraulic head values in the aquifer. Over a span of 125 years, the streamlines would depict the pathways that water particles would have taken from the starting cell towards Well 2. The streamlines may diverge, converge, or follow intricate patterns depending on the aquifer properties, heterogeneity, and the influence of other wells or boundary conditions in the model.

By analysing the streamlines, hydrogeologists can gain insights into the flow pathways and connectivity of the aquifer. This information can be useful for understanding the movement of contaminants, assessing the capture zone of pumping wells, and evaluating the potential impacts of pumping activities on nearby water sources. In summary, the concept of 125 years streamlines refers to tracing the paths of water particles backward in time over a 125-year period. Starting from a specific cell, the streamlines depict the flow pathways towards Well 2, providing insights into the direction and patterns of groundwater flow. These streamlines are valuable for understanding aquifer connectivity, contaminant transport, and evaluating the impact of pumping wells on the aquifer system.

Conclusion

The results obtained from the PMPATH model, which generated steady-state head distributions and capture zones of pumping wells. Figure 3 shows the steady-state head distribution in the first model layer, representing the spatial distribution of hydraulic head values. Contour maps of hydraulic heads display the groundwater levels in the aquifer system, with lower contours indicating areas near pumping wells where drawdown is greatest. These maps provide insights into groundwater flow patterns, well influence zones, and aid in groundwater management. Figure 4 presents the steady-state hydraulic head distribution in the third model layer and shows the capture zones of pumping wells. The capture zone refers to the area from which groundwater is drawn into the well, influenced by hydraulic gradients and hydraulic head distribution. Analysing flow paths and gradients helps understand groundwater behaviour and make informed decisions regarding well placement and groundwater management.

The forward particle tracking simulation introduces a contaminant source upstream of Well 2 to observe its movement through the steady-state flow field over different time periods. Figure 5 displays the streamlines representing the paths water particles would follow in the groundwater system over 125 years. Starting from cell [6, 5, 1], the streamlines trace the paths backward in time towards Well 2. The direction of streamlines is influenced by hydraulic gradients, aquifer properties, and other factors. Analysing streamlines provides insights into flow pathways, connectivity of the aquifer, contaminant transport, and the impact of pumping wells on nearby water sources. In summary, the PMPATH model generated steady-state head distributions, capture zones of pumping wells, and streamlines to understand groundwater flow patterns, aquifer connectivity, and contaminant transport. These findings contribute to groundwater management and decision-making processes.

Acknowledgement

The research focuses on riverbank filtration (RBF) technology and the simulation of contaminant transport in a riverbank filtration system using a two-dimensional model. It considers factors like velocity, dispersion, adsorption, and decay of contaminants. The finite difference method (FDM) is utilized to solve the contaminant transport equation. The study investigates the impact of hydraulic conductivity and the distance between contamination source and pumping well. It emphasizes the need for a model to simulate contamination behavior and understand parameters influencing contaminant transit in groundwater systems. The methodology explains the use of the FDM and mentions the MODFLOW software as an example. It discusses the advantages of the FDM, including simplicity, mass conservation, and numerical extensions. The advection dispersion reaction (ADR) equation is introduced to describe solute transport, and the mathematical formulation presents the equations for the contaminant transport model, considering adsorption and the balance equation for concentration. The results and discussion section discusses the steady-state head and hydraulic head distributions obtained from MODFLOW simulations. It explains their significance in understanding groundwater flow patterns and capture zones of pumping wells. The forward particle tracking simulation is described as a method to observe contaminant movement over time and analyze streamlines to understand flow pathways and aquifer connectivity.

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