Numerical Simulation of Contaminant in Transient Groundwater System

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Abstract

This work aims to study the transportation of contaminants in a groundwater system, which is one of important problems in environmental science. The study relies on numerical simulations of a system of partial differential equations; the transport equation for contaminant flow and transient groundwater flow. The numerical methods are handled by the discontinuous Galerkin (DG) method for spatial coordinates, and together with the second order two-stage Alexander scheme for the time evolution system. The implementation for the simulations is performed based on DUNE library. The study of contaminant is considered with and without pump and treat (P&T) techniques, where the simulation results are provided via examples together with accuracy validation of the numerical method.

Keywords: Discontinuous Galerkin, Contaminant Transportation, Transient Groundwater
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1 Introduction

Groundwater contamination is one of the major environmental issues that treatens to global water resources and human health. According to a survey of the United States Geological Survey, approximately one of five tested groundwater wells have at least one chemical contaminant [1] which are hazadous to daily consumption. Therefore, to address this issue, factors such as the type of groundwater flow, the properties of the aquifer, and the techniques used to treat the contaminants are considered when developing a mathematical model to predict the future scenario.

Mathematical models are essential tools to simulate a complex phenomenon, such as the transport of contaminants in groundwater. One commonly used model is the advection-diffusion equation, which describes the mechanism of contaminant transport in groundwater; however, this equation cannot explain the influence of external factors like a changing in groundwater velocity. To address this limitation, the transient groundwater equation is applied, as it accounts for time-varying flow. The connection between these two equations is described by a groundwater hydraulic head gradient, which represents a spatial change in the hydraulic head and relates to the advection term in the contaminant transport equation.

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Since the governing equations are a system of partial differential equations (PDEs), numerical methods, such as the Finite Element Method (FEM) and Discontinuous Galerkin (DG) method are commonly employed to solve them. The FEM is a widely used numerical technique for simulating groundwater contaminant in domain with irregular geometries. For instance, one of the first models that applied this method to solve the coupled system of both two equations was developed by Yeh [2] in 1981. Building upon this, Khebchareon [3] extended this approach by developing a two-dimensional finite element to solve the coupled system of the steady-state groundwater flow equation and the advection-dispersion equation. Similarly, Smaoiu [4] impremented an FEM code to solve transient groundwater in heterogeneous media.

Since groundwater contamination models must effectively capture advection-dominated transport to provide reliable predictions, to address this challenge, the Discontinuous Galerkin (DG) method is introduced for solving this problems. The Discontinuous Galerkin (DG) method, introduced in the 1970s, employs discontinuous piecewise polynomial approximations to achive high orders of accuracy and has proven effective for advection-dominated problems [5]. In 2003, Wheeler et al. [6] applied this method to simulate a far-field nuclear waste management problem. Subsequently, Dawson, Sun, and Wheeler [7] investigated a system of equations in which the transport algorithm is compatible in 2004. Later, Povich [8] extended its application to coupled equations with variable density in 2012.

Regarding groundwater contaminanation remediation, the most commonly used method is the Pump and Treat (P&T) technique [9]. This technique is the groundwater well established approach involves extracting contaminanted water, transporting it to a designated treatment area, and then discharging the treated water back into the groundwater system. For example, in 2008, Sharief et al [10] applied this concept to optimize the pumping rate for cleaning up a confined aquifer with FEM. Additionally, Ahmadi et al [11] investigated the effect of pumping rate on treating contaminant groundwater with Finite Volume Method (FVM).

From these advantages in both numerical methods and remediation techniques, this study investigates the effectiveness of the P&T method for remediating contaminant transport within an anisotropic aquifer under transient ground waterflow condition. The numerical simulations are handled by the discontinuous Galerkin (DG) method for spatial coordinates, and by the second order two-stage Alexander scheme for the time evolution system.

2 Contaminant Flow in Groundwater Model

In this simulation, for more real-world realistic mathematical model, the governing equations are the advection-diffusion equation and the transient groundwater flow equation. The advection-diffusion equation describes the transport of contaminant caused by the advection and diffusion processes in the groundwater system, and this equation is derived from the conservation of mass law. For spatial space $(x, y) \in \Omega \subset \mathbb{R}^2$, and temporal space $t \in [0, T)$, let a function $c(x, y, t)$ be the contaminant concentration in the groundwater. The advection-diffusion equation can be expressed in mathematical as:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) - \nabla \cdot (D\nabla c) = f_c, \tag{2.1}$$

where $\mathbf{u}(x, y, t)$ is the groundwater velocity, $D(x, y)$ is the diffusion coefficient, and f_c is contaminant source or sink function.

The transient groundwater flow equation explains the groundwater movement. This equation is derived from Darcy's law and continuity equation. For a saturated porous media, let $h(x, y, t)$ be a hydraulic head function. The transient groundwater flow equation can be written as follows [12]:

$$S_s \frac{\partial h}{\partial t} - \nabla \cdot (K \nabla h) = f_h, \tag{2.2}$$

where S_s is the specific storage coefficient, $K(x, y)$ is the hydraulic conductivity coefficient, and f_h is the groundwater source or sink function.

The groundwater velocity $\mathbf{u}$ in equation (2.1) can be expressed in the gradient respected to a spatial domain by using the Darcy's law:

$$\mathbf{u} = -\frac{K \nabla h}{\phi}, \tag{2.3}$$

where a constant ϕ is the aquifer porosity.

To build the general system of the mathematical model, let $\Omega \subset \mathbb{R}^2$ be a bounded domain, $\partial\Omega = \Gamma_D \cup \Gamma_N$ be the boundary of Ω which is subjected to Dirichlet boundary (Γ_D) and Neumann boundary (Γ_N), and n be the outward unit normal vector. The governing equations can be written as:

$$\begin{aligned}
\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) - \nabla \cdot (D \nabla c) &= f_c && \text{for } \Omega \times (0, T), && (2.4)\\
S_s \frac{\partial h}{\partial t} - \nabla \cdot (K \nabla h) &= f_h && \text{for } \Omega \times (0, T), && (2.5)\\
c(x, y, t) &= g_c && \text{on } \Gamma_D \times (0, T), && (2.6)\\
h(x, y, t) &= g_h && \text{on } \Gamma_D \times (0, T), && (2.7)\\
\frac{\partial c}{\partial n} &= 0 && \text{on } \Gamma_N \times (0, T), && (2.8)\\
\frac{\partial h}{\partial n} &= 0 && \text{on } \Gamma_N \times (0, T), && (2.9)\\
c(x, y, 0) &= c^0 && \text{on } \Omega, && (2.10)\\
h(x, y, 0) &= h^0 && \text{on } \Omega, && (2.11)
\end{aligned}$$

where g_c and g_h is contaminant concentration and hydraulic head corresponded to Dirichlet boundary condition, and c^0 and h^0 is the initial for concentration and hydraulic head, respectively.

3 Numerical Methods

For numerically solving the system of governing equations, the governing equation is changed to a weak form. Let $H^1(\Omega)$ be the Sobolev space defined by

$$H^1(\Omega) := \left\{ f \in L^2(\Omega) : \partial f \in L^2(\Omega) \right\}, \tag{3.1}$$

where $L^2(\Omega)$ is the space of square integrable functions and ∂f is the first order weak derivative of the function f. Let Ψ and Ξ denote the Sobolev spaces for contaminant concentation function

$c(x, y, t)$ and hydraulic head function $h(x, y, t)$, respectively. For test functions $\psi \in \Psi$ and $\xi \in \Xi$, weak forms of equations (2.4) to (2.11) are:

$$\int_\Omega \frac{\partial c}{\partial t}\psi dx + \int_\Omega \nabla \cdot (c\mathbf{u})\psi dx + \int_\Omega D\nabla c \cdot \nabla \psi dx + \int_{\Gamma_D} g_c \psi ds = \int_\Omega f_c \psi dx, \tag{3.2}$$

$$\int_\Omega S_s \frac{\partial h}{\partial t}\xi dx + \int_\Omega K\nabla h \cdot \nabla \xi dx + \int_{\Gamma_D} g_h \xi ds = \int_\Omega f_h \xi dx. \tag{3.3}$$

In this study, the Discontinuous Galerkin method (DG) is used to solve the governing equation in spatial domain. Let $\mathcal{T}_h$ be the finite element mesh consisting of elements T, and let $\mathcal{E}_h$ be the set of all element interfaces. The notations $(\cdot,\cdot)_{\mathcal{T}_h}$ and $(\cdot,\cdot)_{\mathcal{E}_h}$ represent the discrete L^2 inner products with respect to $\mathcal{T}_h$ and $\mathcal{E}_h$, respectively. Then, the semi-discrete scheme is written as

$$\begin{aligned}\left(\frac{\partial c_h}{\partial t}, \psi\right)_{\mathcal{T}_h} &= (c_h\mathbf{u}, \nabla\psi)_{\mathcal{T}_h} - \left((c_h^{up}\mathbf{u}) \cdot n, [\psi]\right)_{\mathcal{E}_h} - (D\nabla c_h, \nabla\psi)_{\mathcal{T}_h} \\ &\quad + (\{D\nabla c_h \cdot n\}, [\psi])_{\mathcal{E}_h} + (f_c, \psi)_{\mathcal{T}_h},\end{aligned} \tag{3.4}$$

$$\left(S_s\frac{\partial h_h}{\partial t}, \xi\right)_{\mathcal{T}_h} = -(K\nabla h_h, \nabla\xi)_{\mathcal{T}_h} + (\{K\nabla h_h \cdot n\}, [\xi])_{\mathcal{E}_h} + (f_h, \xi)_{\mathcal{T}_h}, \tag{3.5}$$

where $c_h^{up}\mathbf{u}$ is an upwind flux, $\{v\}$ is an average of function v, and $[v]$ is a jump of v.

Let $\{t_n\}_{n=0}^N$ be the discrete time points partitioning the interval $[0, T]$, with a time step defined as $\Delta t = t_{n+1} - t_n$. The contaminant concentration and hydraulic head at time t_n are denoted by c^n and h^n, respectively. For time discretization, the second-order and two stage Alexander scheme which known as a diagonally implicit Runge-Kutta (RK) method [13] is applied to discretize the time domain. This scheme provides a stability, making well-suited for numerical solution of the governing equations. The general implicit equation, for solving the contaminant concentration c of the next time step is given by

$$c_1^n = c^n + \alpha\Delta t f(t_n + \alpha\Delta t, c_1^n), \tag{3.6}$$

$$c_2^n = c^n + \Delta t(1-\alpha) f(t_n + \alpha\Delta t, c_1^n) + \alpha\Delta t f(t_n + \Delta t, c_2^n), \tag{3.7}$$

$$c^{n+1} = c^n + \Delta t(1-\alpha) f(t_n + \alpha\Delta t, c_1^n) + \alpha\Delta t f(t_n + \Delta t, c_2^n) \tag{3.8}$$

where α is a weight which equals to $1 - \dfrac{\sqrt{2}}{2}$.

4 Numerical Experiment

In this study, the Distributed and Unified Numerical Environment (DUNE) is used to implement the governing equations, by using the DG scheme with the second order and two stage Alexander scheme, to the programming language. DUNE is a free and open toolbox based on C++ language for the grid-based numerical imprementation such as fininte element (FEM), finite volume (FVM), or discontinuous galerkin (DG) methods [14]. The computational setup includes an Intel i7-12700 processor with 16 GB of RAM, and equilateral rectangle element for the mesh.

The model parameters for all simulations in this study are shown in Table 1.

Table 1: Input data for all simulations

Parameters	Value
Diffusion coefficient ($D(x, y)$)	5.46×10^{-8} m^2/s
Specific storage coefficient (S_s)	1
Hydraulic conductivity ($K(x, y)$)	2.69×10^{-6} to 1.3×10^{-3} m/s
Aquifer porosity (ϕ)	1
Time step (Δt)	1 day (86400 s)
Final time (T)	2000 days
Domain (Ω)	$[0, 100]^2$ m^2
Element dimension ($\Delta x, \Delta y$)	1 m $\times$1 m

To represent the heterogeneity of an aquifer, the hydraulic conductivity ($K(x, y)$) is generated by randomization from a log-normal distribution, defined by the equation

$$K(x, y) = \exp\left(Y(x, y)\right), \tag{4.1}$$

where $Y(x, y)$ is a Gaussian random field which is the normal distribution with mean -9.5 and varriance 1. To simulate the anisotropic aquifer, the correlation lengths are set to 20 m. in the x-direction and 5 m. in the y-direction. Basesd on these setting, the aquifer is represented to be a mixture of clay and fine sand, with the range of hydraulic conductivity is approximately 2.69×10^{-6} m/s to 1.3×10^{-3} m/s [15,16]. Figure 1 shows the result of the randomized hydraulic conductivity used in model simulation.

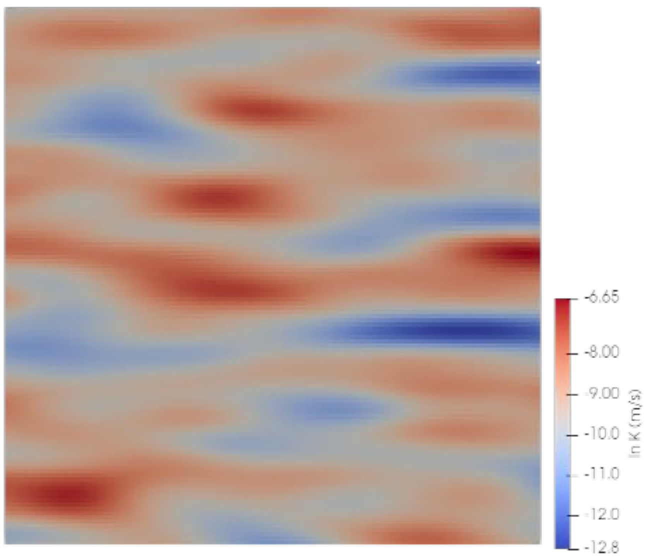


Figure 1: Aquifer texture generated by randomized hydraulic conductivity

4.1 Accuracy Validation

In this section, the model validation is discussed to study the accuracy of numerical solutions for the contaminant concentration function $c(x, y, t)$. Since this problem does not have an analytical solution, a convergence of numerical solution is performed. The numerical solution should converge to the numerical solution from the finest mesh. The finest mesh, $h = 0.00125$ meter with sufficiently small time step $\Delta t = 1$ day is used as a benchmark for comparing the numerical solutions obtained from the coarser mesh sizes. The compared mesh size that used in this study are $h = 0.02, 0.01, 0.005$, and $h = 0.0025$ meter.

For the accuracy validation, let $c_h(x, y, t)$ be the contaminant concentration for the mesh size h at grid point (x, y), $E_{max}(c_h)$ be a discrete maximum norm, $E_{L^2}(c_h)$ be a discrete L^2 norm, and $\mathrm{EOC}(h_i)$ be an order of convergence which define by the following definitions:

$$E_{max}(c_h, t) = \max_{(x,y)\in\Omega_h} |c_{exact}(x, y, t) - c_h(x, y, t)|\,, \tag{4.2}$$

$$E_{L^2}(c_h, t) = \sqrt{\frac{\sum\limits_{(x,y)\in\Omega_h} (c_{exact}(x, y, t) - c_h(x, y, t))^2}{n_h}}, \tag{4.3}$$

where n_h is the number of grid point in Ω_h and

$$\mathrm{EOC}(h_i) = \frac{\log(E_{h_{i-1}}/E_{h_i})}{\log(h_{i-1}/h_i)}, \tag{4.4}$$

where E_{h_i} denotes the maximum error over time $t \in [0, T]$ for E_{max} and E_{L^2} with mesh size h_i.

The validated model is configured to simulate contaminant transport in transient flow, as described in Example 4.1.

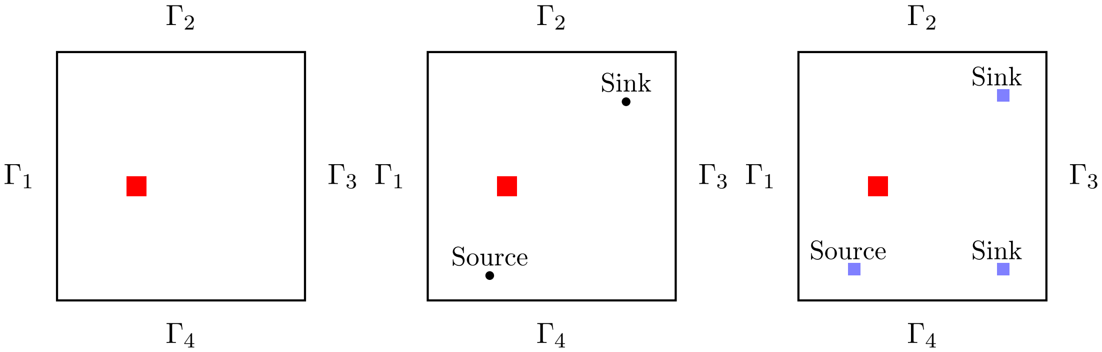
Example 4.1 (Contaminant in transient flow).

In this example, the boundary for the hydraulic head of groundwater h is set to 1 m. on Γ_1 and 0.8 m. on Γ_3. The other boundaries are set to be Neumann boundary conditions which the net flux equals to zero. For the contaminant concentation, the boundary condition is set to outflow boundary. The initial plume is defined on $(28, 36) \times (42, 50)$ with a concentration 1 mg/L (see Figure 2a).

Table 2: Errors and rates of order of convergence for example 4.1

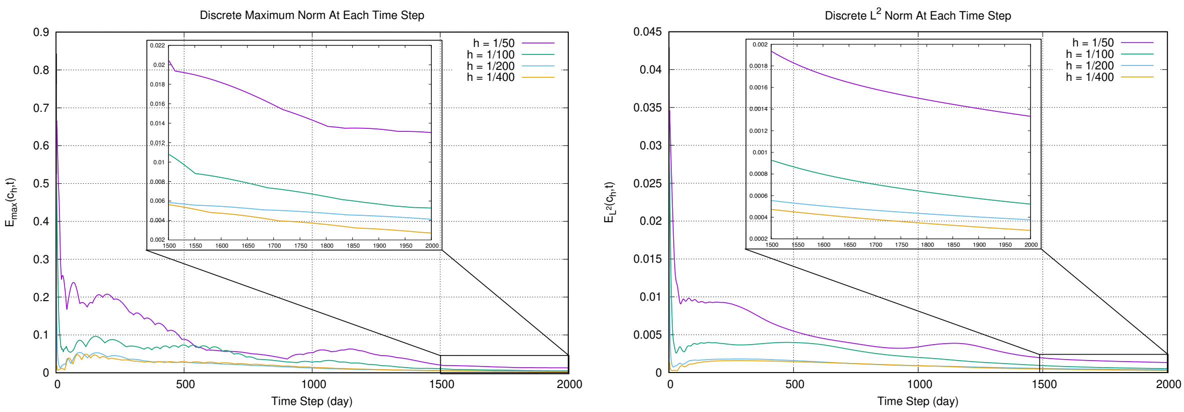
h	$E_{max}(c)$	$\mathrm{EOC}(h_i)$	$E_{L^2}(c)$	$\mathrm{EOC}(h_i)$	Time (sec)
0.02	0.8435	-	0.0429	-	206
0.01	0.7619	0.1468	0.0395	0.1191	1065
0.005	0.5249	0.5376	0.0290	0.4458	6386
0.0025	0.1556	1.7542	0.0103	1.4934	45557

From the Table 2, both errors measured by E_{max} and E_{L^2} decrease as the mesh size h decreases. This suggests that the simulations converge and stable when finer grids are used, which validate the accuracy of the method (see also Figure 3a and 3b); however, these smaller

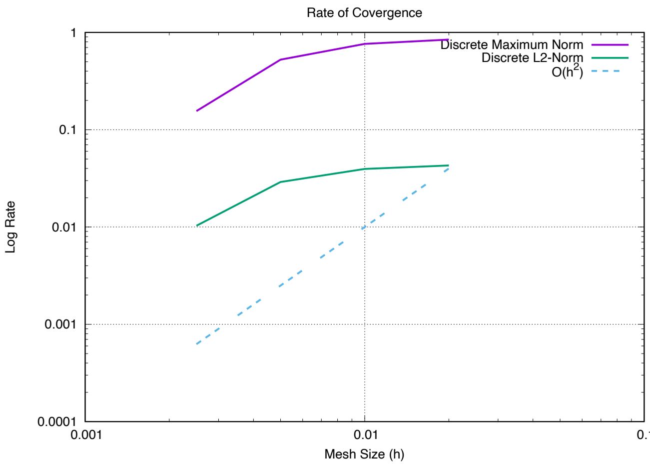


(a) (b) (c)

Figure 2: (a) Problem domain for groundwater pollutant with no treatment, (b) a single-point P&T technique, and (c) a regional zone P&T technique



(a) (b)

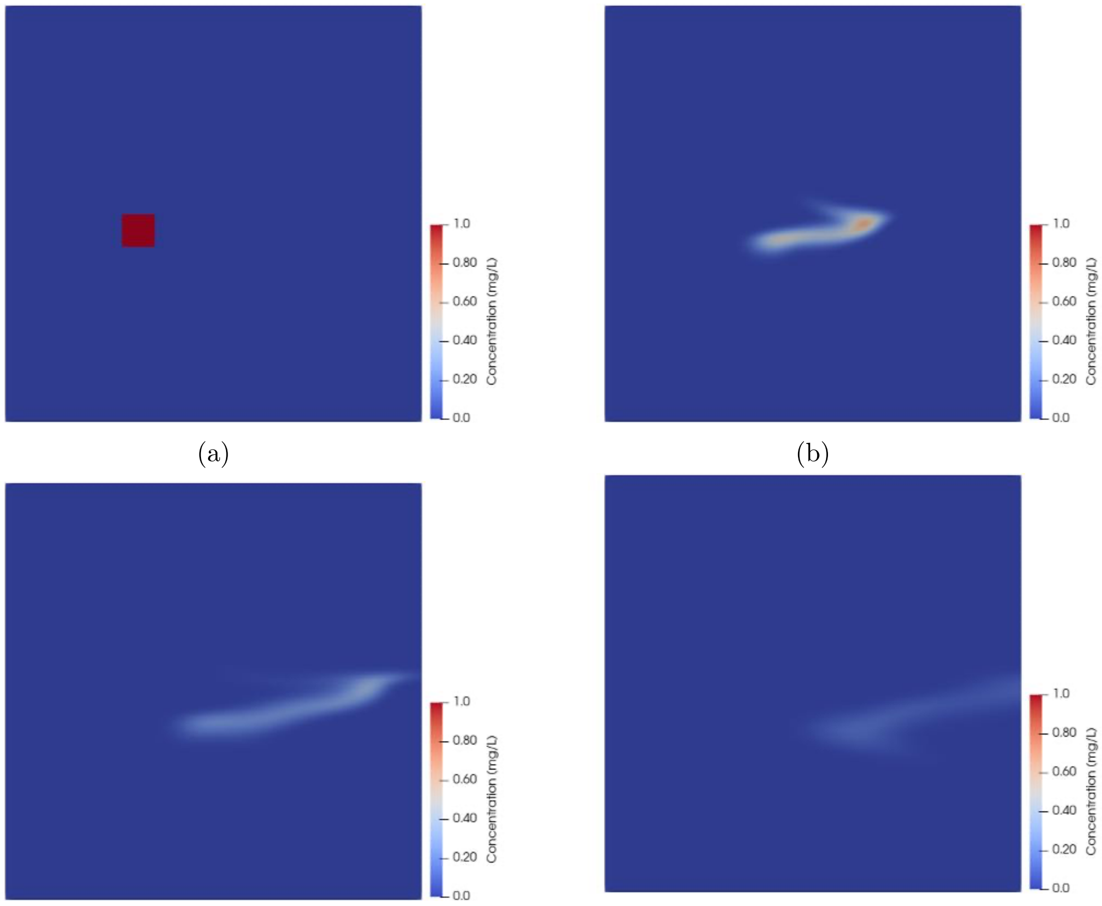


(c)

Figure 3: (a) Discrete maximum norm, (b) L^2 norm, and (c) rate of convergence of Example 4.1

grid sizes require more processing time for simulation. Moreover, as shown in Figure 3c, The EOC is approximately predicted to follow $O(h^2)$ as the grid size h decreases.

Figure 4 shows the simulations results for contaminant concentration at different times. The contaminant appears on the source of the contaminant at the initial time (Figure 4a), and then transports away from the source by the groundwater flow (Figure 4b and 4d), where the spreading of the plume (a high concentration of contaminant region) is influenced by the hydraulic of conductivity. Figure 5 illustrates that simulated velocity field at various times; at the initial time, the flow is relatively uniform (Figure 5a). As time progresses the flow paths are distinct (Figure 5b), and the velocity field of groundwater reaches a steady state around 120 days where the velocity field seems to be identical (see Figure 5c and 5d).



(a) (b)

(c) (d)

Figure 4: (a) Pollutant flow at time $t = 0$ day, (b) 500 days, (c) 1000 days, and (d) 2000 days

4.2 Simulations of Groundwater Contamination Remediation with P&T technique

This study aims to investigate groundwater contaminant treatment, the Pump and Treat methods (P&T). Two simulation scenarios; single point and region zone, are presented for analyzing a behavior of contaminant extraction in groundwater system.

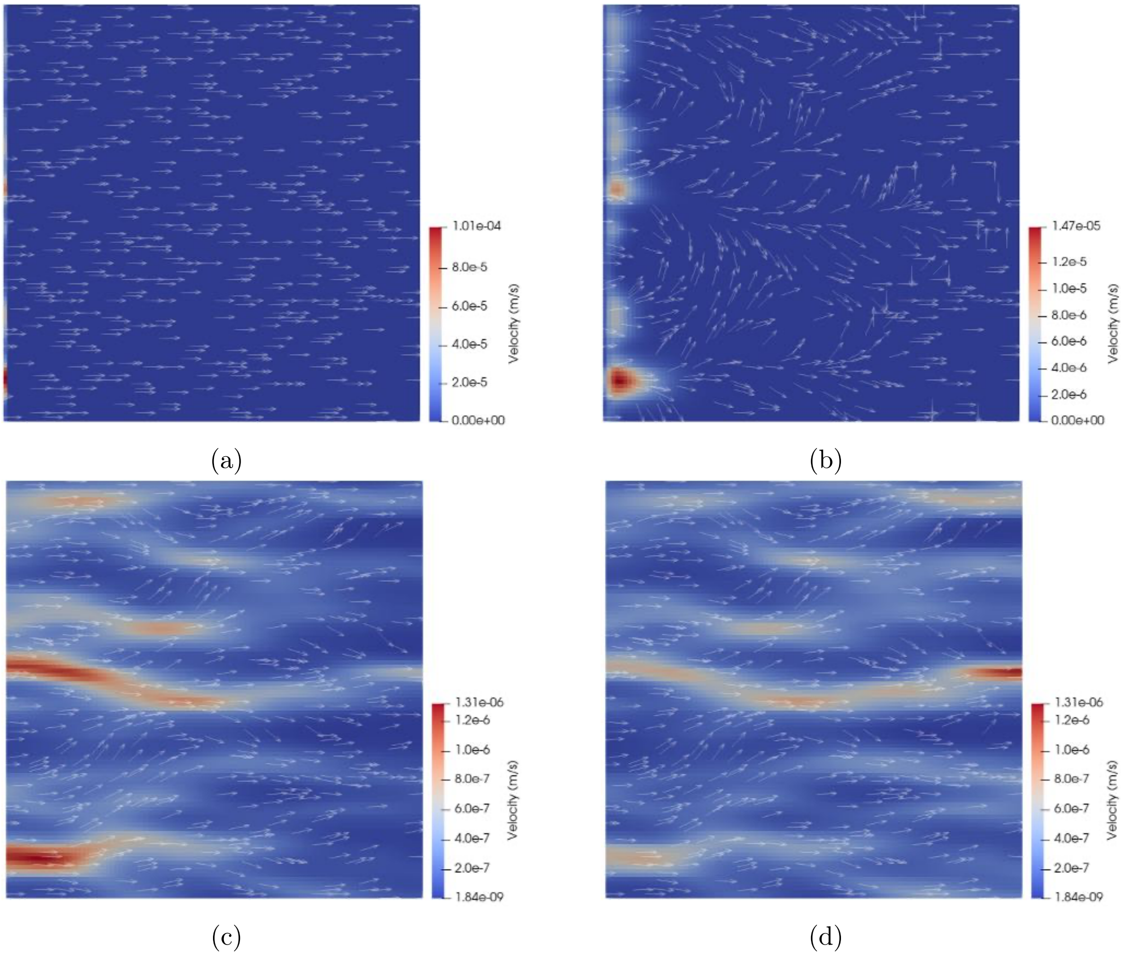


Figure 5: (a) Velocity field at time $t = 0$ day, (b) 1 day, (c) 120 days, and (d) 2000 days

Example 4.2 (P&T with points sink and source).

In this example, the effect of a single-point P&T technique is studied. One groundwater source point and one groundwater sink point are added to the studied area, the domain Ω, and operated throughout the simulation continuously. As shown in Figure 2b, the source point is set up at $(25, 10)$ with the rate of injection 9.25×10^{-5} m^3/s, and the sink point is set up at $(80, 80)$ with the rate of extraction 1.01×10^{-5} m^3/s.

Figure 6 demonstrates that the groundwater sink effectively removes contaminants from the system. As illustrate in Figure 6c, the concentration drops significantly to 0.003 mg/L at 1000 days and further decreses to 4×10^{-6} mg/L at the day 2000 (Figure 6d). This reduction is due to the high velocity of groundwater source, which pushes the contaminant towards the sink point. Figure 7 shows how the source point influences the flow pattern of groundwater, which reaches to a steady state after 120 days (see Figure 7c and 7d).

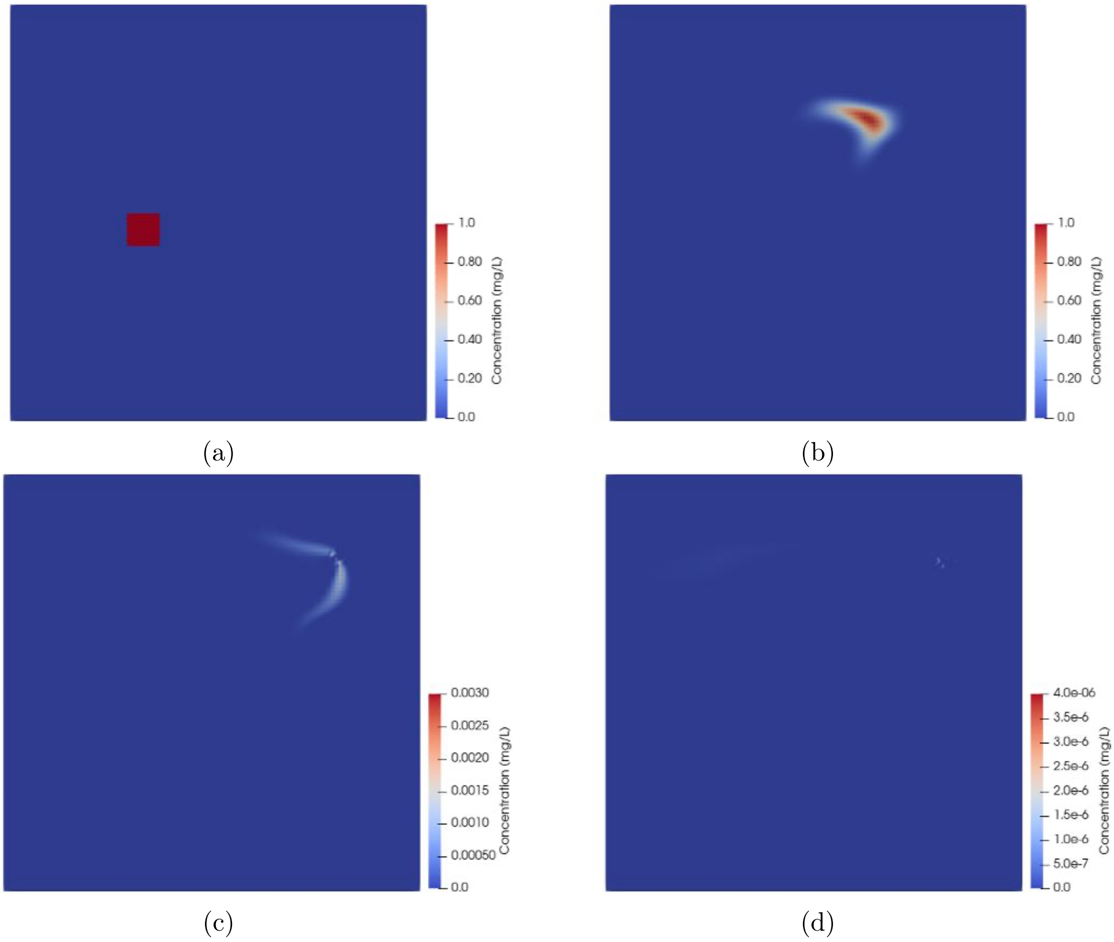


Figure 6: Contaminant concentration at time $t = 0$ day (a), 500 days (b), 1000 days (c), and 2000 days (d)

Example 4.3 (P&T with regions sink and source).

In this example, the sink and source point have replaced by region zones with dimension 5×5 m^2. and another sink region zone has added in the domain Ω, as shown in Figure 2c. Parameters for each zone are given in Table 3 .

Table 3: Parameters for simulation in example 4.3

Parameters	Source	Sink1	Sink2
Position	$(20, 25) \times (10, 15)$	$(80, 85)^2$	$(80, 85) \times (10, 15)$
Rate (m^3/s)	9.25×10^{-5}	1.01×10^{-5}	6.01×10^{-5}
Hydraulic conductivity (m/s)	1×10^{-3}	1×10^{-3}	1×10^{-5}

Figure 8 show that the sink region can remove the contaminant from the system. As shown in Figure 8b, the plume is advected from the contaminant source towards the right size of the

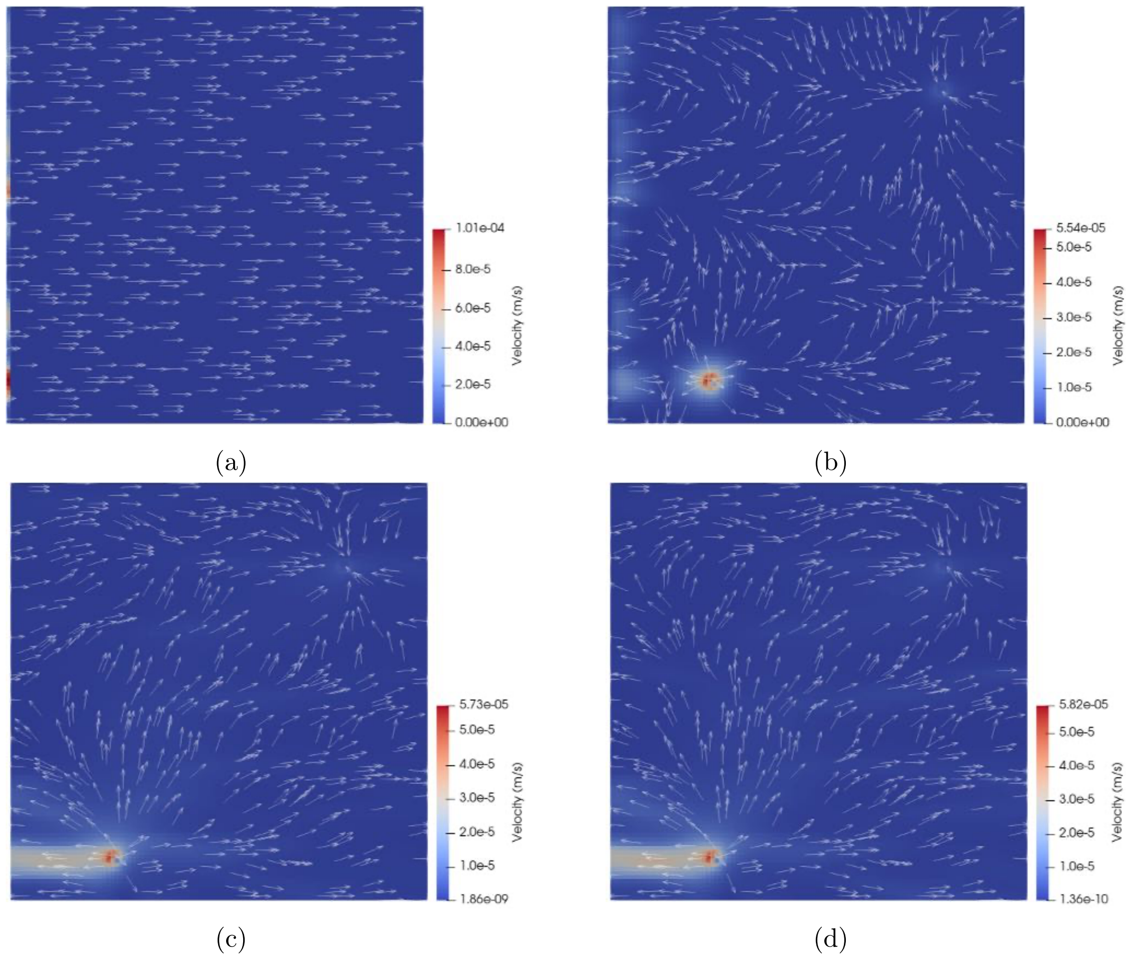


Figure 7: Velocity field at time $t = 0$ day (a), 1 day (b), 120 days (c), and 2000 days (d)

domain due to groundwater velocity from the source region; while most of contaminant flows out of the system, some is extracted by the sink regions. The upper-right sink appears to be more effective at contaminant removal than the bottom-right sink, as illustrate in Figure 8c and 8d.

5 Conclusion

In this study, the Discontinuous Galerkin (DG) method, combined with a two-stage, second-order Alexander scheme, is used to solve a coupled system of the advection-diffusion equation and the transient groundwater flow equation. The numerical solution for the concentration function $c(x, y, t)$ is obtained through an implementation in the DUNE library. Moreover, the inclusion of the transient term in the groundwater flow equation, along with the use of randomized hydraulic conductivity values, contributes to a more realistic simulation. The accuracy of the simulation is evaluated using the discrete maximum norm and discrete L^2 norm is computed following to the approximation in the second order. The Pump and Treat (P&T) technique is applied to the model for remediating contaminant groundwater. The simulations show that a strategically

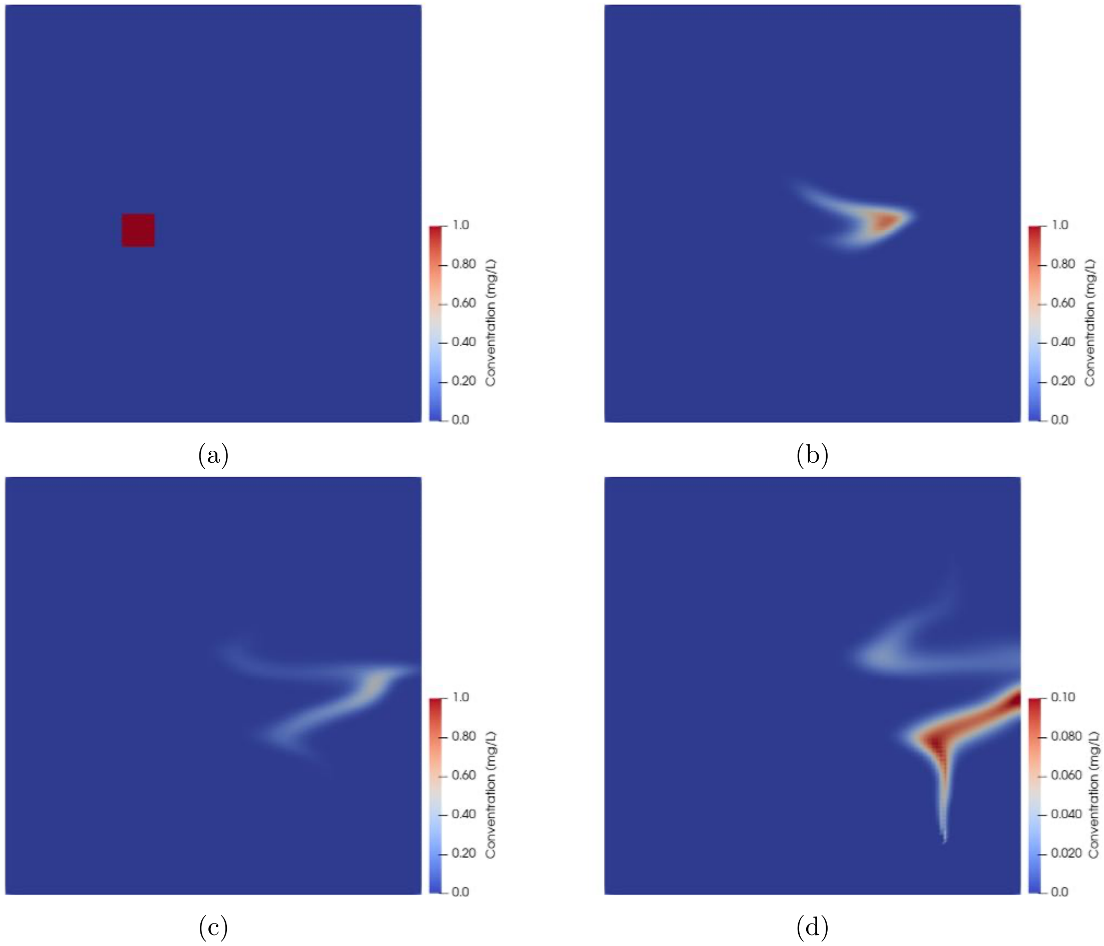


Figure 8: (a) Contaminant concentration at time $t = 0$ day, (b) 500 days, (c) 1000 days, and (d) 2000 days

placed groundwater source can drive the contaminant plume towards a groundwater sink, leading to significant contaminant removal and a reduction in overall concentration within the system.

This simulation can help decision-makers predict the movement of the contaminant and design efficient groundwater well locations and optimal pumping rates to minimize operational costs and timelines. Future studies could explore using the real-world data or coupling the model with optimization algorithms.

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