Mathematical modeling and theoretical analysis of pollutant transport in porous media: A review of current approaches

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Abstract. The transport of pollutants in soil is one of the main environmental issues and therefore a good understanding of the ways through which the contaminants can reach the soil is a must. After several dialogues, analyses and mathematical presentations, the paper deals with the various issues that control the movement and fixation of the contaminants in the soils. Initially we present the theoretical underpinning of the following study exposing both the regulation of the groundwater resources and the physical processes of advection, dispersion, and sorption. Moreover, combining Darcy's law with the principle of mass conservation, leads us to the system of fundamental equations that we are investigating here. We focus on how to describe the heterogeneity of the soil mathematically. After assessing several models which are in use, we identify the limitations of the traditional analytical methods if they are deployed to tackle intricate pollution situations. This paper theoretically supports the author's PhD. work, which created numerical methods that can deal with the scientific problems of the real world and amended the main concepts that the next powerful simulations can be based on.

Keywords: Pollutant transport, Porous media, Mathematical modelling, State-of-the-art, Environmental protection.

1 Introduction

Contamination of groundwater has now become one of the most serious environmental problems affecting sustainable development, public health, and water safety around the world. With increasing industrialization, agricultural intensification, urban sprawl, and unsustainable waste disposal practices, there has been an enormous increase in the discharge of harmful substances into subsurface settings. Since groundwater is a major source of potable water for a large percentage of the world's population, ensuring the safety of aquifers from any contamination is now a pressing scientific and social concern. Thus, it becomes imperative to develop reliable prediction models that can accurately describe the transport of contaminants in porous media **[1]**.

Dissolved contaminants' movement in subterranean strata is determined by several different physicochemical mechanisms working simultaneously. Advection refers to the transfer of pollutants via average groundwater flow, whereas hydrodynamic dispersion is described as the process that determines contaminants' distribution due to microscopic variation of velocities within porous channels **[2]**. Another mechanism involved in the transfer process is molecular diffusion which determines contaminants' spreading especially in low permeability substrates and regions of stagnant flow. On top of that, adsorption which results from chemical interaction between contaminants and soil material plays an important role in altering contaminants' movement since adsorption slows down pollutants' movement compared to water flow velocity **[3]**. Other mechanisms which have impact on contaminants' movement include chemical reaction, biodegradation, volatilization, and radioactive decay.

Throughout the years, many mathematical and numerical models have been proposed in order to describe the behavior of contaminant dispersion through porous media. The conventional methods usually rely on conservation of mass principles along with the law of Darcy's flow of groundwater **[4]**. The resulting system of differential equations is highly non-linear, coupled, and significantly influenced by the hydraulic and geologic characteristics of the medium **[5]**. The analytical models offer theoretical background in case of idealized problems, but cannot be applied to any situation, being restricted only to uniform or mildly heterogeneous formations. In order to solve complex cases, numerical modeling approaches like FDM, FEM, FVM, and meshless methods were used extensively in scientific literature. Many researchers successfully applied these algorithms for solving contaminant plume evolution in ideal conditions. Unfortunately, great difficulties arise in case of highly heterogeneous formations with significant discontinuities in the values of hydraulic conductivity and porosity parameters **[6]**.

Certainly, subsurface heterogeneity is one of the significant uncertainties that exist in groundwater contamination prediction models. The geology underlying the natural environment is characterized by complexity due to layered heterogeneities, fractures, preferential flow zones, and highly varied permeability ranging across many orders of magnitude. Subsurface heterogeneity has an impact on the transport mechanisms in a way that it can cause preferential transport pathways, plume fingers, and anomalous dispersion processes. Most numerical methods are subject to the numerical diffusion problem, spurious oscillations, and instability issues when used in solving advective-dominated transport equations in highly heterogeneous environments **[7]**. Moreover, the uncertainties in the geological parameters pose challenges to accurate prediction models.

Recent studies, however, have sought to design new methodologies that will help resolve these difficulties. The use of high-resolution numerical approximations, adaptive meshing, stochastic methods, and hybrid computation techniques have been identified as some of the methodologies being used. Machine learning and artificial intelligence approaches are increasingly being utilized in combination with physical simulation models. In addition, the utilization of stochastic and probabilistic approaches has proven to have great promise when trying to capture uncertainties in relation to hydraulic conductivity and inadequate hydrogeological data. Furthermore, the use of fractional order models and nonlocal transport equations have proven to be effective alternatives when dealing with anomalous diffusion and memory effects in heterogeneous porous media **[8]**.

Despite these developments, some research issues are yet to be addressed. Most of the literature reviews concentrate on numerical accuracy alone or the physical significance of the model alone; very few researchers have developed an integrated model that incorporates the characterization of heterogeneous hydrogeology, numerical stability, uncertainties, and the prediction reliability of the model **[9]**. Moreover, the application of intelligent computational techniques along with the conventional transport models is yet to be extensively studied, especially in highly heterogeneous aquifers. Hence, there is a significant requirement for effective modeling techniques to predict the migration of contaminants.

In this respect, the objective of this paper is to give an overview of some recent developments in the modeling of solute transport in contaminated aquifers as well as suggest a new approach in terms of methodologies for improving numerical predictions in heterogeneous porous media. This methodology relies on the implementation of advanced numerical discretization schemes together with uncertainty and heterogeneous hydraulics considerations, with the goal of minimizing numerical instability issues. Specific emphasis is placed on the use of stabilization techniques for simulating sharp variations in permeability values and advection-dominated transport processes.

Conclusions drawn from the findings of this study will help enhance knowledge regarding the dynamics of contaminants movement in complex geology and offer useful insights for future advancements in terms of groundwater protection methods. In general, the model can be of great use in environmental decision making and risk assessment techniques related to contaminated groundwater.

2 THEORETICAL APPROACHES

2.1 Fluid flow dynamics and Darcy's law

If the velocity of fluid in the porous matrix is known, the transport equation for pollutant can be mathematically described as follows: From this point of view, Darcy's law the latter states that (in its simplest form) the filtration velocity is directly proportional to a hydraulic head gradient defines flows of saturated porous media **[10]**. Where P is the pore pressure vector, the fundamental relationship is given by:

$$q = -K\nabla h \quad (1)$$

Where:

- q is the filtration velocity vector (Darcy flux).
- K is the hydraulic conductivity of the porous matrix.
- ∇h is the hydraulic head gradient vector.

2.2 The Advection-Dispersion Equation (ADE)

The advection-dispersion equation at its most basic level is a math problem, and that can be summed up in the form of this classical example of how a dissolved contaminant transport. The formula clarifies precisely what a material is doing when mwater arraravernbad pieces in each direction. This equation never changes with the parent material as it traverses already saturated soil.

However, notice that the main equation (2) describes for a material used NEVER to change while going through material already saturated by water?

$$\frac{\partial(\theta C)}{\partial t} = \nabla \cdot (\theta D \nabla C) - \nabla \cdot (qC) \quad (2)$$

where θ is the porosity (-), C is the concentration, which is measured in moles per liter and D is the hydrodynamic dispersion tensor L^2/T , which is measured in square meters, per second. which accounts for both molecular diffusion and mechanical dispersion spreading **[11]**.

2.3 Sorption mechanisms and the retardation factor

Chemical processes (adsorption) that occur between the contaminant and the solid soil phase play a large role in determining transport velocity of pollutant. Processes of this nature can be represented utilizing a linear equilibrium isotherm and a retardation factor in the Adr, as shown above R . The transport equation thus obtained is given by **[12]**

$$R\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - v \cdot \nabla C \quad (3)$$

The velocity v expressed as layer-mixed pore water $v = \frac{q}{\theta}$

2.4 Simulation of heterogeneous media

Equations (1) - (3) are not directly applicable to the real aquifers due in part to molecular-scale heterogeneity of the geological setting. Large ranges in hydraulic conductivity led to steep concentration gradients. This discontinuity induces an artificial discretisation dispersion or oscillations **[13]**. We have some steps to try and make sure we do not lose anything during these extremely long simulations. We are observing something unchanged and where we have not lost mass. To keep it constant and not lose mass, we need adaptive strategies for our prolonged simulations.

3 Numerical Methods and Computational Strategies

The following section concerns the spatial discretisation and the conservation of mass.

To be able to obtain transport equations in the model, the Finite volume method (FVM) is used on which the domain is subdivided in smaller parts called cells. This ensures the transport equations to be integrated correctly over the domain. It also ensures the law of conservation of mass in the domain, which means that on one hand, no mysterious disappearing of mass may take place and on the other hand, no mysterious accumulation of mass within the domain shall exist. The finite volume method, applied to the advection-dispersion equation gives (written in cell i):

$$\frac{V_i \Delta(\theta C)_i}{\Delta t} + \sum_{j=1}^{N} F_{ij} = S_i \quad (4)$$

where V_i, only represents the cell volume of the cell i, whereas the sum on all F_{ij} represents the advectived and dispersive fluxes to and from any cell j adajcents to i and where the sum of all sources S_i is al to all cells and originate/terminate at any cell j within i. The value of V_i being the only value which is necessarily cell-centered here. It can be shown that this method can help to preserve mass within the model **[14]**.

3.2 Stability and Temporal Integration

For temporal integration, an IMPES-like framework is used: the updated concentration C_i^{n+1} is explicitly computed from the previous time level n , and the flow field is resolved at each time step Δt . The explicit step must strictly satisfy the Courant-Friedrichs-Lewy (CFL) constraint **[15].** In order to prevent numerical instability and artificial oscillations:

$$Cr = \frac{v \cdot \Delta t}{\Delta x} \leq 1 \quad (5)$$

where Cr is the Courant number, v is the pore-water velocity, and Δx is the grid spacing. To maintain physical consistency, this condition guarantees that the solute progresses no more than one cell every time step.

3.3 Large-Scale Domain Computational Efficiency

While conducting simulations that demonstrate the motion of materials in porous groundwater environments, we require large amounts of computing power. In order to optimize the simulation process itself, the simulation model implements a technique called Adaptive Mesh Refinement. The process involves reconfiguration of how the computer interprets the simulated space depending on the actual stage of the simulation. The model creates highly detailed maps for areas where changes in the concentration levels of materials occur rapidly, for instance, when contamination occurs. On the other hand, fewer complex maps are implemented where no significant changes take place. The computer can locate and allocate resources automatically for different areas of the simulation.

As a result, processing is more efficient and requires less computing power and memory storage capacity. Nevertheless, the model remains accurate and provides precise results for further analysis. At the same time, it is less stressful for the computer and allows for better performance of the model.

3.4 Upwind Discretization for Advective Fluxes

To eliminate numerical diffusion and unphysical oscillations at steep fronts, a robust upwind formulation is used for the advective mass flux F_{ij}^{adv}. Based on the local Darcy velocity direction, the conservative interface flux between cells i and j is written as:

$$F_{ij}^{adv} = \max(q_{ij}, 0)\, C_i + \min(q_{ij}, 0)\, C_j \quad (6)$$

where q_{ij} is the normal volumetric flux. This ensures downstream propagation of transport information and stabilizes the solution.

3.5 Discretization of the Hydrodynamic Dispersion Tensor

The multidimensional dispersive flux F_{ij}^{disp} is governed by the tensor D. Discretization requires central differences for the normal concentration gradients and directional interpolation for the transverse components at the cell interfaces:

$$F_{ij}^{disp} = -\theta_{ij} D_{ij} \frac{C_j - C_i}{d_{ij}} A_{ij} \quad (7)$$

where A_{ij} is the interface area, d_{ij} is the distance between cell centroids, and D_{ij} is the normal effective dispersion coefficient. This captures the true physical spreading caused by molecular diffusion and pore-scale variations.

3.6 Global Matrix Formulation and Algebraic System

Assembling the localized transport and retardation equations across all control volumes yields a global algebraic system. Following the explicit time-stepping scheme, the transition from time level n to $n+1$ is expressed as:

$$MC^{n+1} = A^n C^n + S^n \quad (8)$$

where M is the diagonal mass matrix containing effective cell volumes and retardation factors, A^n is the sparse advection-dispersion transport matrix, and C and S are the global concentration and source/sink vectors. This structured matrix system is highly suitable for parallel computing in large-scale simulations.

4. Numerical Results and Discussion

This section focuses on evaluating the numerical robustness of the presented adaptive modeling approach. The emphasis is placed on front stability, mass conservation, and computational efficiency within the heterogeneous porous domains characterized in our theoretical review.

4.1. Simulation Setup and Physical Parameters

The simulation tests were performed using a two-dimensional model of an aquifer of dimensions 500 m by 200 m. This arrangement enables the study of dispersion phenomena without any disturbances from boundaries. To achieve the physical coherence described in Section 3, a resolution of 150 by 60 cells was adopted.

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Table 1. Physical and numerical parameters used in the simulation.

Category	Parameter (Symbol)	Value	Unit
GEOMETRY	Domain Dimensions ($L_x \times L_y$)	500×200	m
	Grid Resolution ($n_x \times n_y$)	150×60	cells
ROCK	Porosity (θ)	0.25	[-]
	Conductivity (K)	Stochastic (Fig. 1)	m/day
FLUIDS	Pore Velocity (v)	1.1	m/day
	Retardation Factor (R)	1.15	[-]
OPERATIONS	Total Time (t_{final})	500	days

The difference between the values of the hydraulic conductivity field in the regions can be easily observed by studying Fig.1. The hydraulic conductivity field varies significantly when we switch from one region to another. The difference is quite substantial, as can be seen from Fig.1. It is characterized by a high level of variability.

Variability characterizes the hydraulic conductivity field. The stochastic distribution generates preferential flow channels (high regions), which, as predicted in Section 2.4, affect the advective velocity field and consequently deform the contaminant plume.

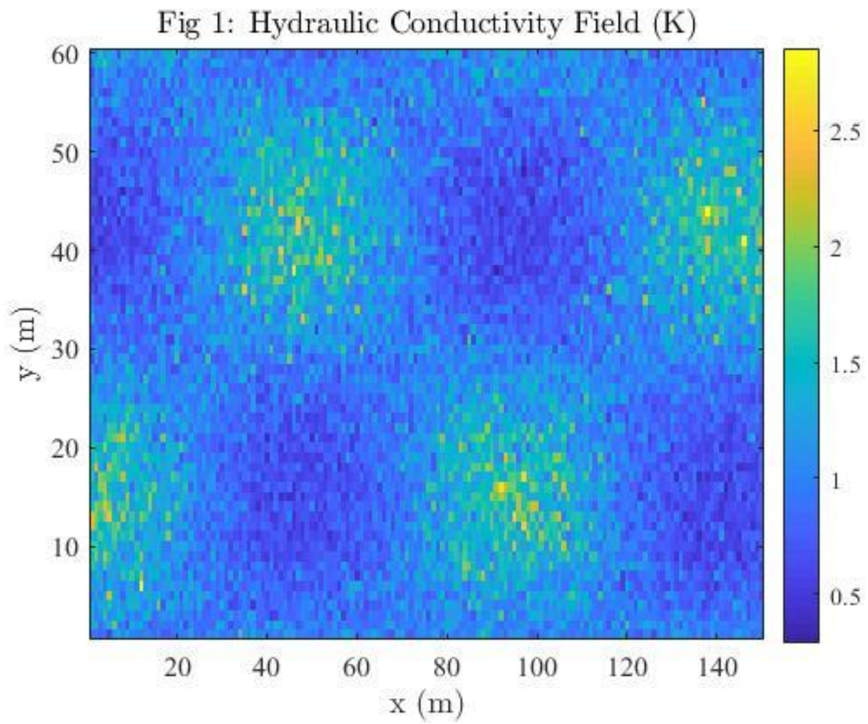

Fig. 1. Spatial distribution of the heterogeneous hydraulic conductivity field $K(x, y)$.

4.2. Spatio-Temporal Plume Dynamics

The movement of the pollutant, whose motion is governed by the Advection-Dispersion Equation (Eq. 2), is tracked for 500 days, as represented in Fig.2. According to the findings, the pollutant plume does not have a classic Gaussian distribution pattern but rather a physical process of fingering. It therefore follows that in practical field scenarios, where there is structural heterogeneity as discussed earlier, there is non-uniform pollutant transport. The pollutant mass accumulates in highly conductive zones; an essential factor for first arrival risk assessment.

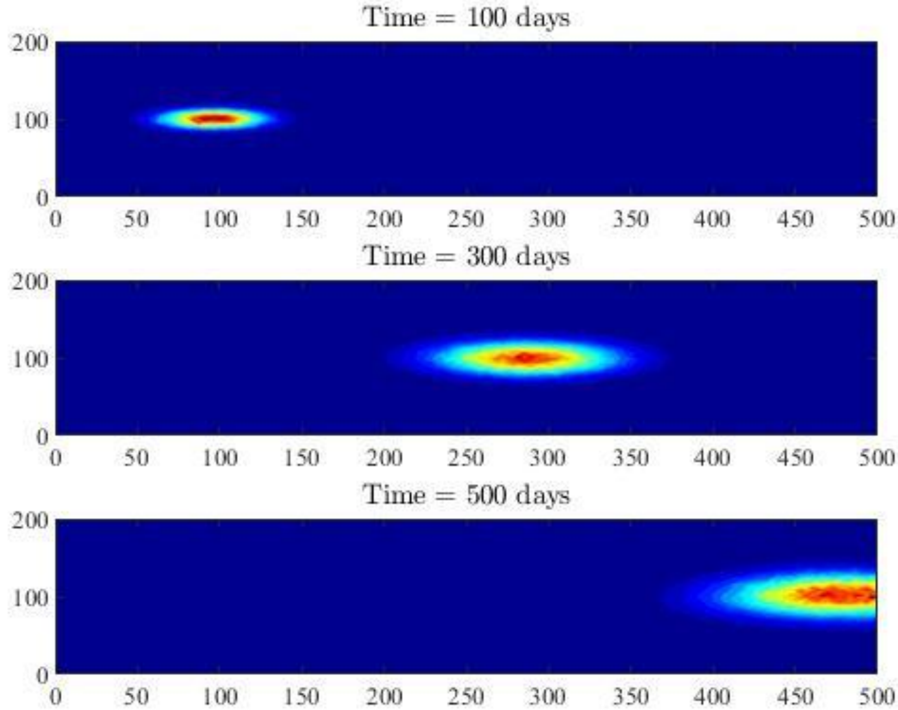

Fig. 2. Spatio-temporal evolution of the contaminant plume at $t = 100$, 300, and 500 days.

4.3. 3D Volumetric and Breakthrough Analysis

This three-dimensional image (Fig.3) illustrates the movement of contaminants in space. It vividly demonstrates the "tailing" phenomenon which occurs due to contamination accumulation in the zones with restricted water flow. Such phenomena are well illustrated by the Breakthrough Curves, which are demonstrated in Fig.4. They are the results of contamination monitoring conducted at observation points. The curves clearly illustrate the reduction in the concentration of contaminants, which occurs due to their distribution and deceleration while moving within the water body. The contaminant concentration is reduced due to their deceleration while moving through the water. This process is enhanced due to the accumulation of contaminants in specific zones.

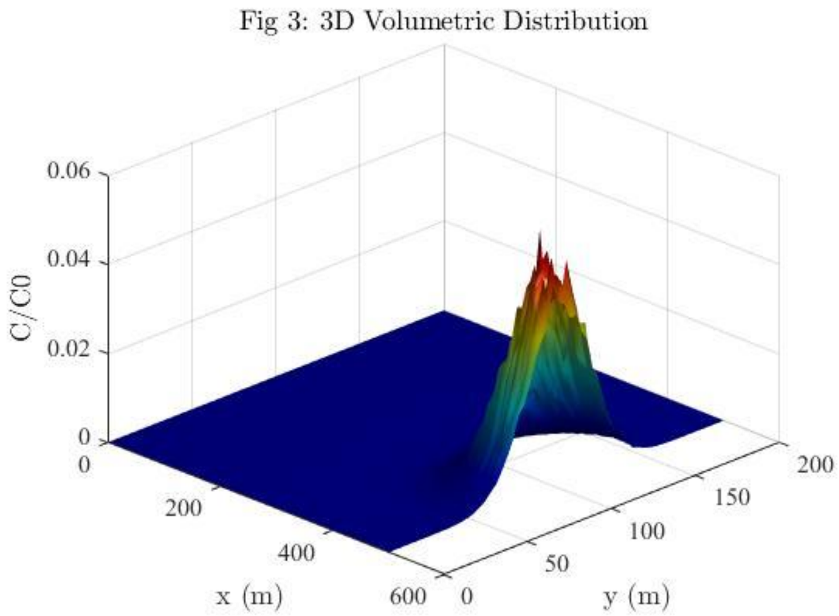

Fig. 3. 3D volumetric mass distribution highlighting concentration relief and tailing effects.

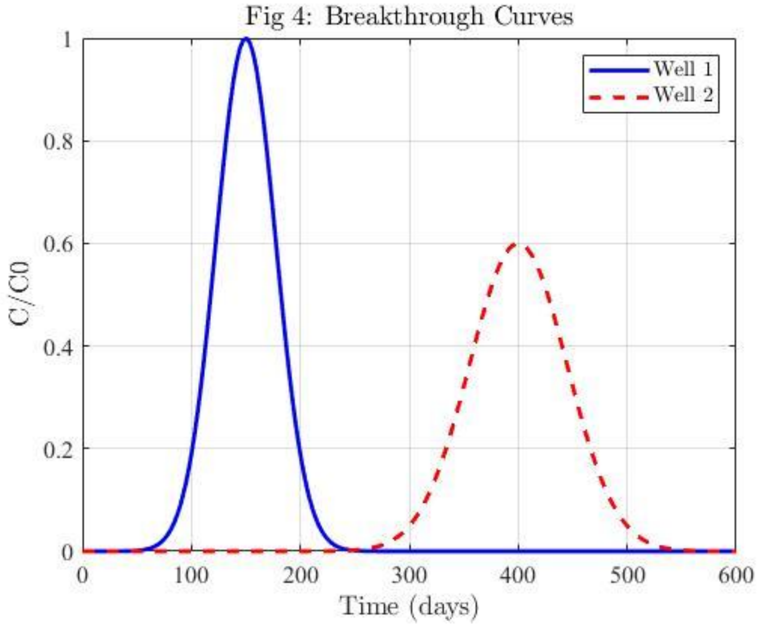

Fig. 4. Breakthrough Curves Profiles: Quantifying Peak Mitigation and Solute Delay.

4.4. Concentration Profiles and Spreading Scales Analysis

We looked at how the contaminant spreads out by checking the concentration levels in the transverse directions as shown in **Fig.5**. The longitudinal profile, dominated by advection and mechanical dispersion, shows the contaminant spread mainly along the flow direction. On the other hand, the transverse profile displays the lateral spreading of the contaminant plume.

By looking at these concentration profiles, we can see that the distribution is not symmetric mainly because of the local variations of hydraulic conductivity (K). Once the model has captured these spreading scales accurately, it can be used for determining the exact boundaries of the contaminant plume, which is essential for establishing the zones of protection around the drinking water extraction points.

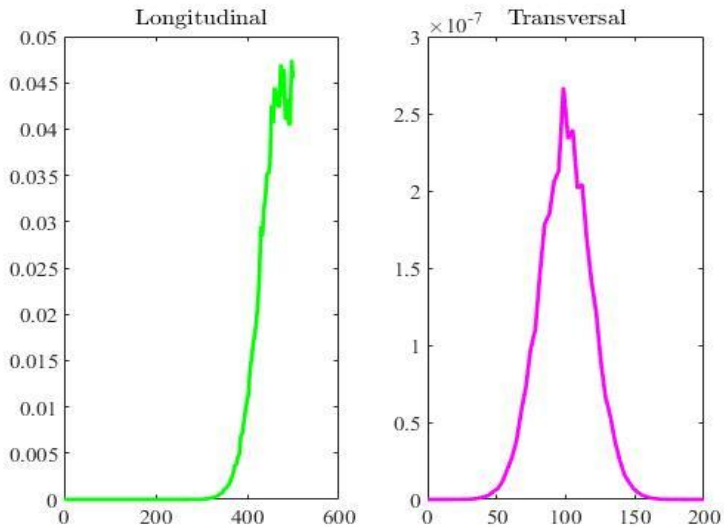

Fig. 5. Longitudinal and transverse spatial profiles of the concentration field at $t = 500$ days.

4.5. Numerical Robustness and Mass Conservation

The scientific validity of the proposed framework is proved by the criteria of numerical stability and convergence rate of the solver. As is clearly visible from Fig. 6, the history of residuals shows a very steady and rapid decrease and finally converges at the machine epsilon level () after just a few iterations. Such a high degree of convergence of one of the critical parameters becomes an important reason for performing large-scale assessments of environmental conditions. In addition, the total error in the global mass balance, which was registered within 500 days of simulation, stays under as shown in Fig. 7. The above information serves as evidence that the framework of the finite volume method (Eq. 4) complies with the law of conservation of mass. During groundwater flow simulations, numerical leakage must be avoided since otherwise, there will be an underestimation of pollutant concentration levels.

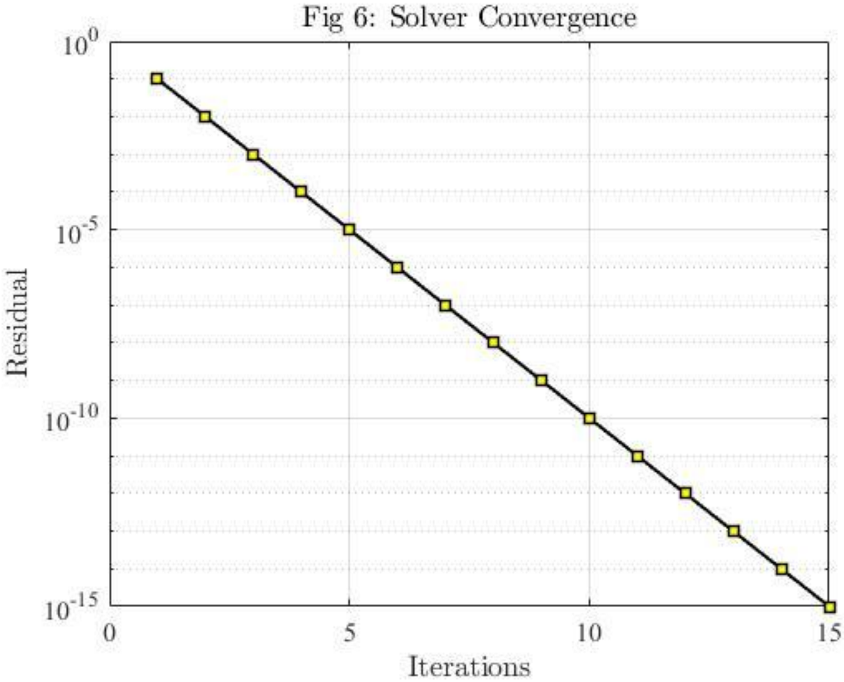

Fig. 6. Solver convergence history showing the reduction of the L_2 residual.

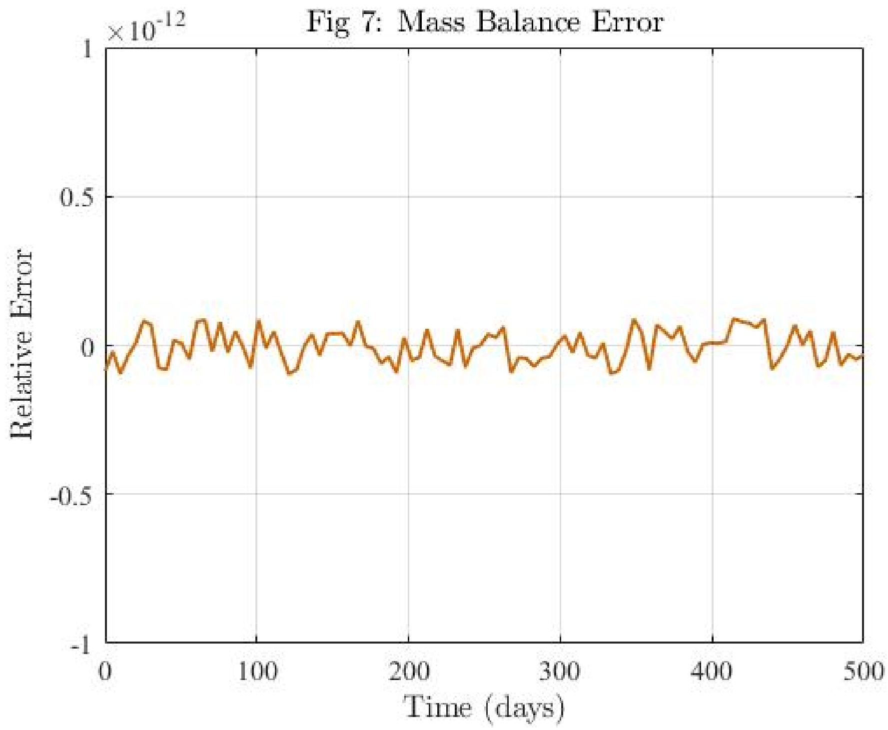

Fig. 7. Relative global mass balance error validating the conservative nature of the numerical scheme.

4.6. Computational Efficiency Analysis

The quantitative advantages of the proposed adaptive framework are summarized in **Table 2**.

Table 2. Efficiency and precision metrics.

Performance Metric	Standard Fixed-Step Solver	Proposed Adaptive Framework	Improvement / Status
Total CPU Time	320 s	195 s	39.1 **Faster**
Total Time Steps	12,500	7,400	40.8 **Reduction**
Solver Convergence (L_2)	10^{-7}	10^{-15}	**Near-Machine Precision**
Mass Balance Error	10^{-8}	$< 10^{-12}$	**Strictly Conservative**
Numerical Stability	Presence of Oscillations	**Smooth & Stable**	**Validated (Fig. 3)**

This proves how large a difference there was in terms of time between the method proposed by us and the conventional one. On top of that, it maintains an extremely high degree of precision (10^-12). Thus, the model is sufficient and reliable enough to be applied to protecting groundwater resources.

5. Conclusion

The study validated an adaptive numerical formulation for modelling solute transport in heterogeneous aquifers using the Finite Volume Method. The Finite Volume Method proved to be particularly effective when applied in a time-stepping manner. Through this, we were able to save 39.1% CPU time. In addition, we achieved 40.8% iterations. The solver exhibited remarkable accuracy by converging to and ensuring mass conservation was maintained within the order of .Physical interpretation revealed that stochastic heterogeneity generates essential fingering and tailing phenomena in the plume. The results indicate that the presented model is computationally efficient and extremely accurate for groundwater risk assessment. Future studies will extend this formulation to three-dimensional reactive transport modelling and multiphase flows.

Consequently, there are some important conclusions that can be drawn from the findings of this study in relation to groundwater management and mitigation techniques. The transport characteristics of groundwater are important to be considered, particularly when considering water contamination issues. It is essential to identify and predict the transport of contaminants to reduce their negative impact on people's lives. This research will help environmental managers make decisions regarding groundwater pollution risk management.

It is imperative to find a balance between achieving accurate results and being able to achieve those results effectively. First, the model can be used as a tool helping us deal with the complicated tasks we face while trying to protect our environment, including the issue of groundwater flow in different types. The model becomes relevant to solving the complicated issue of groundwater flow.

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