# Effects of Dispersion Parameters and Low Permeability Porous Media on the Contaminant Transport Behavior in the Aquifer System: A Numerical Study

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## Abstract

In this study, contaminant transport behaviour in the aquifer system (140 m × 180 m × 5 m) was analyzed using a 3-D groundwater flow and contaminant transport model viz. MODFLOW2005 and MT3DMS. The impacts of hydrodynamic dispersion parameters on the conservative contaminant plume dynamics were analyzed for homogeneous and heterogeneous aquifer systems with low permeability porous media (LPPM). The spatio-temporal distribution of contaminant concentration and breakthrough curves (BTCs) at 12 observation wells were used to analyze the transport dynamics due to conservative contaminant released from a single point source over a hypothetical study area for a period of 1 year (365 days). Results from MODPATH show a significant variation in the pathway of groundwater for homogeneous and heterogeneous aquifer systems. During the source loading period, a very low value of concentration of order 10-9 mg/m3 was observed in the LPPM region. The spatial distribution of contaminant plume for aquifer system with LPPM varied largely as compared to homogeneous aquifer system. The maximum value of concentration in the aquifer with LPPM was found to be ˜40% higher than the homogeneous system after source removal. After the source removal, the maximum value of 1.98 mg/m3 was observed for the homogeneous system at a location away from pumping and extraction well after 730 days; however, for a heterogeneous system with LPPM, the maximum value of 2.57 mg/m3 was observed. An early breakthrough was observed for αL= 54 m as compared to αL= 9 m for homogeneous aquifer system, clearly depicting the effect of longitudinal dispersivity on BTC. However, effects of dispersivity on the rising and falling limbs of the BTC were negligible for heterogeneous aquifer system with LPPM. Further, an impact of LPPM and longitudinal dispersivity on the peak concentration value at observation well (OBS-7) was undistinguishable. The numerical simulations carried out in this study mimic the realistic heterogeneous aquifer conditions and highlighted the relevance of LPPM and associated transport processes on contaminant transport dynamics at field-scale, which was usually overlooked.

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# INTRODUCTION

## *I. Motivation*

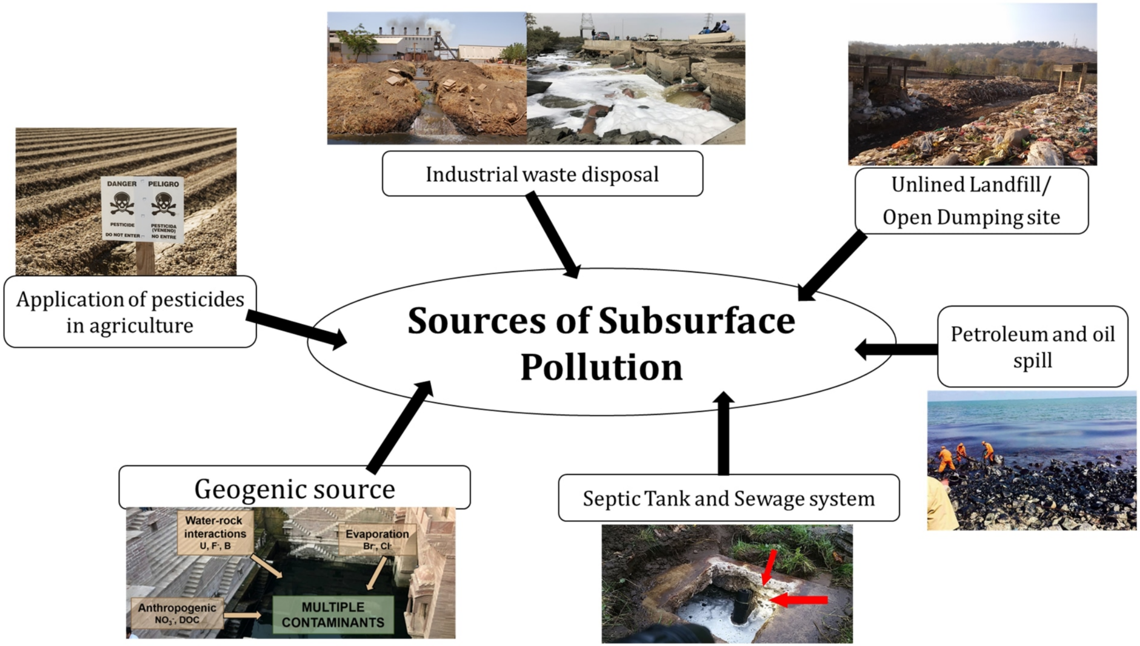


Figure 1: Sources of Subsurface Pollution

- How to determine spatio-temporal variation of contaminant concentration emanating from the above-shown sources at a fine-scale level?
- To understand the impact of flow and transport parameters for homogeneous and heterogeneous aquifer systems.

## *II. Importance of Contaminant Transport Modelling*

- To design remediation operations such as pump and treat method and check the efficacy of operations.
- Design of waste containment facilities such as engineered landfill systems with bottom and side liner.
- To understand complex contaminant transport behavior like the effect of dead-end region, mass-transfer rate, etc.

## *III. Literature survey of studies that emphasized low permeability porous media (LPPM) and dispersion processes*

- Studies indicated that low permeability porous media (LPPM) or aquitard region behave as a sink during contaminant loading period and as a source when the contaminant source is removed or isolated (Chapman and Parker 2005; Chapman et al., 2012; Guo and Brusseau 2017a; Yang et al. 2017a; b).
- LPPM caused long plume tailing for a longer duration due to de-sorption (Brown et al. 2012).

- Non-ideal transport behavior observed for large heterogeneous systems at Tucson International Airport Area (TIAA) federal Superfund site (Guo and Brusseau 2017a; b).

- Non-ideal mass-removal behavior was observed to be governed by back-diffusion from LPPM in the layered or highly heterogeneous aquifer systems (Guo et al. 2019).

Thus, based on the literature, the present study focus on understanding the effects of hydrodynamic dispersion parameters on concentration values for homogeneous and heterogeneous aquifer systems.

# METHODOLOGY

- Contaminant transport behavior in the **aquifer system (140 m × 180 m ×5 m)** was analyzed using a 3-D groundwater flow and contaminant transport model viz. MODFLOW2005 (Harbaugh, 2005) and MT3DMS (Zheng and Wang, 1999).
- The impacts of hydrodynamic dispersion parameters on the **conservative contaminant plume** dynamics were analyzed for homogeneous and heterogeneous aquifer systems with **low permeability porous media (LPPM)**.
- The spatio-temporal distribution of contaminant concentration and breakthrough curves (BTCs) at 12 observation wells were used to analyze the transport dynamics due to conservative contaminant released from a single point source over a **hypothetical study area** for a period of 1 year (365 days).
- Simulations were carried out for 730 days time period.

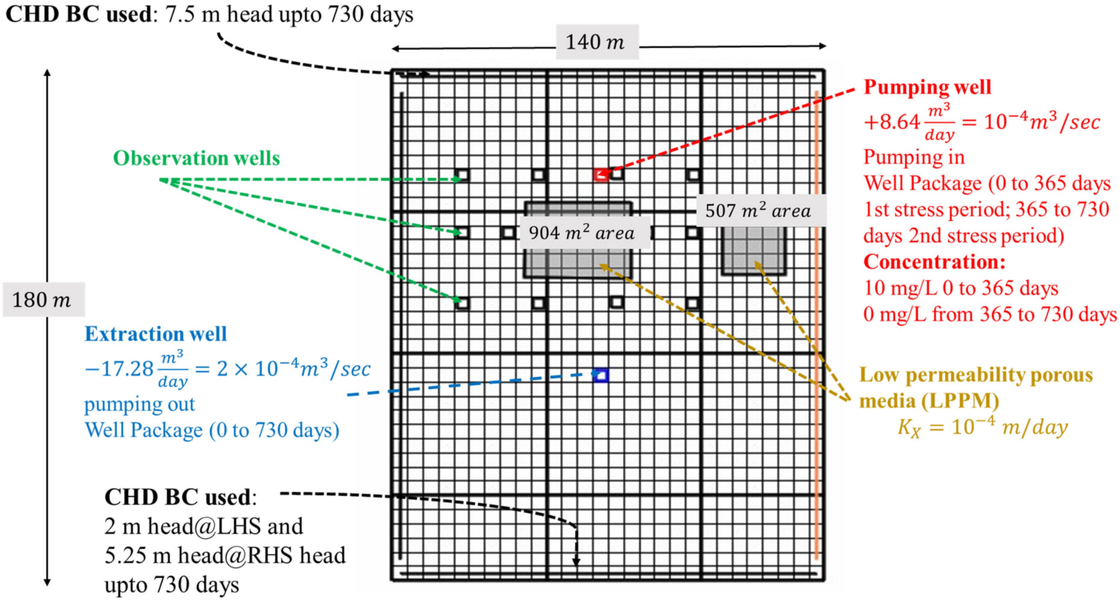


Figure 2: Description of the geometry of numerical model and input parameters

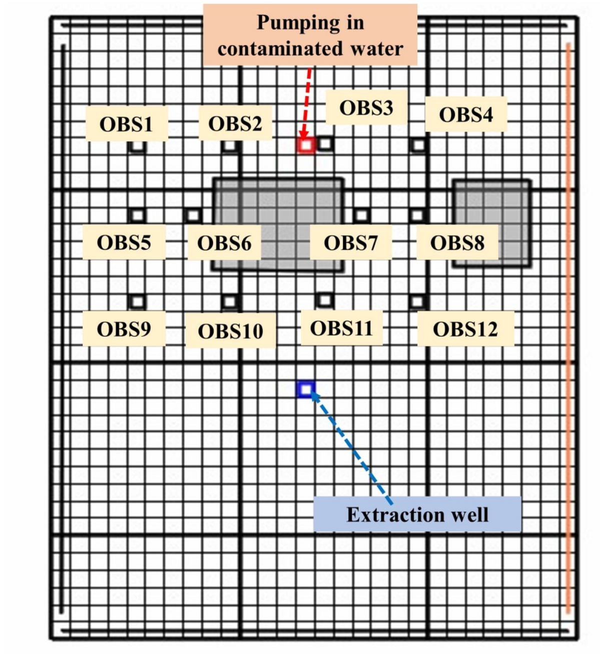


Figure 3: Details of the observation, pumping, and extraction wells

ModelMUSE graphical user interface was used to conduct numerical simulations (Winston, 2020).

### *(I) Details of the packages used for contaminant transport modeling*

- Flow package: Layer property flow package (LPF)
- CHD: Time-variant specified head package
- WEL: Well package for pumping and extraction wells
- Flow solver: SIP (Strongly implicit procedure package)

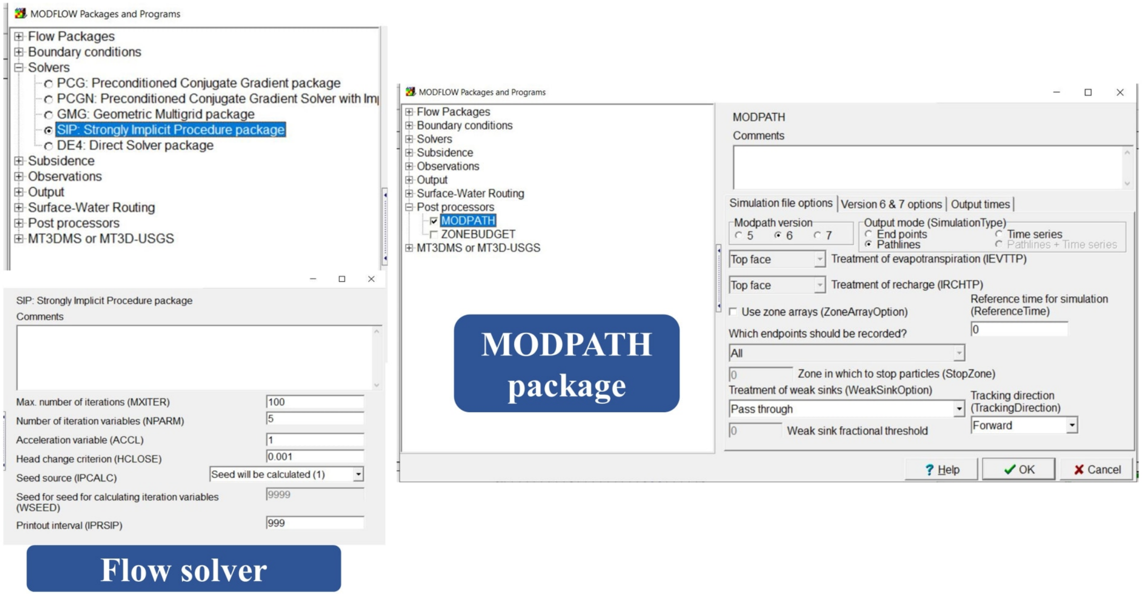


Figure 4: Details of flow solver and MODPATH

## *(II) Transport Package used in MT3DMS via MODELMUSE*

(1) BTN: Basic Transport package

(2) ADV: Advection package

- Advection solution scheme: Standard finite difference method
- Particle tracking algorithm: RK only near sinks/sources
- Weighting scheme: Upstream weighting

(3) DSP: Dispersion package

(4) SSM: Sink and Source Mixing package

(5) GCG: Generalized Conjugate Gradient Solver

- Modified Incomplete Cholesky Preconditioner
- Convergence criteria 1E-06
- Maximum of outer iterations:1
- Maximum inner iterations: 200

## *Details of input parameters used in the study:*

The details of input parameters such as pumping rate, source concentration, hydraulic conductivity of LPPM, etc., are shown in Figure 3.

Depth of aquifer layer = 5 m (single layer)

$K_x$ (aquifer region) = 1.0 m/day

$K_y$ (aquifer region) = $K_x$

$K_z$ (aquifer region) = $K_x/10$

Porosity = 0.32

Table 1: Input parameters used in the sensitivity analysis

| Scenario | Analysis of scenario | Aquifer system with or without low permeability porous media (LPPM) | $\alpha_L$, Longitudinal dispersivity | $\alpha_{TH}/\alpha_L$ |
|---|---|---|---|---|
| A1 | Effect of $\alpha_L$ and LPPM | LPPM absent | 9 m (5% of 180 m) | 0.2 |
| A2 | | LPPM absent | 18 m (10%) | 0.2 |
| A3 | | LPPM absent | 36 m (20%) | 0.2 |
| A4 | | LPPM absent | 54 m (30%) | 0.2 |
| B1 | Effect of $\alpha_L$ and LPPM | LPPM present | 9 m (5% of 180 m) | 0.2 |
| B2 | | LPPM present | 18 m (10%) | 0.2 |
| B3 | | LPPM present | 36 m (20%) | 0.2 |
| B4 | | LPPM present | 54 m (30%) | 0.2 |
| A2 | Effect of $\alpha_{TH}/\alpha_L$ with and without LPPM | LPPM absent | 18 m (10%) | 0.2 |
| A5 | | LPPM absent | 18 m (10%) | 0.5 |
| A6 | | LPPM absent | 18 m (10%) | 1.0 |
| B2 | Effect of $\alpha_{TH}/\alpha_L$ with and without LPPM | LPPM present | 18 m (10%) | 0.2 |
| B5 | | LPPM present | 18 m (10%) | 0.5 |
| B6 | | LPPM present | 18 m (10%) | 1.0 |

# RESULTS

## (I) Contaminant plume evolution in the homogeneous aquifer system

**Groundwater system without LPPM (Scenario A1)**

**Input Parameters**
$\alpha_L = 9\ m$
LPPM absent

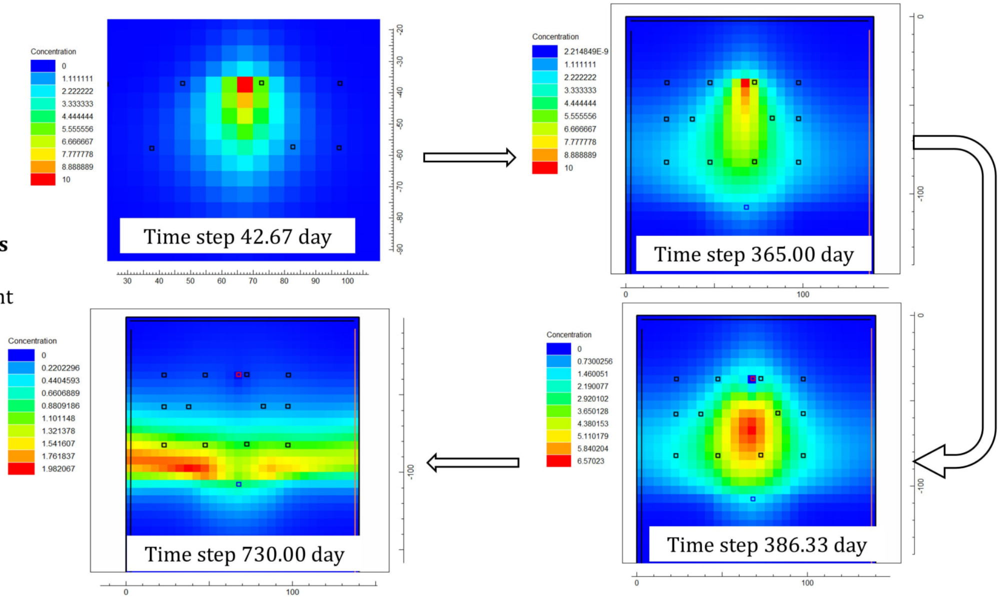

Figure 5: Contaminant plume evolution in the homogeneous aquifer system up to 730 days time level

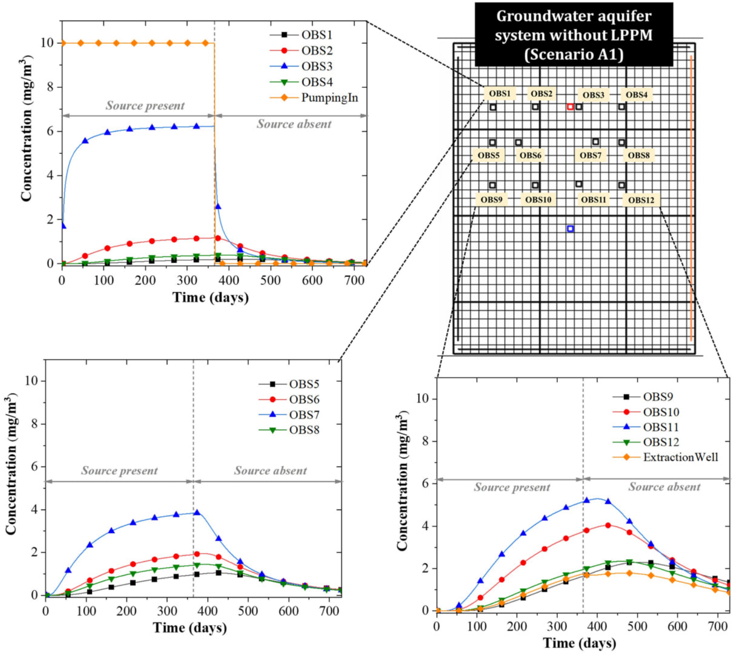


Figure 6: Breakthrough curves(BTCs) predicted at various observation wells

## (II) Comparison of contaminant plume evolution in the homogeneous and heterogeneous aquifer system

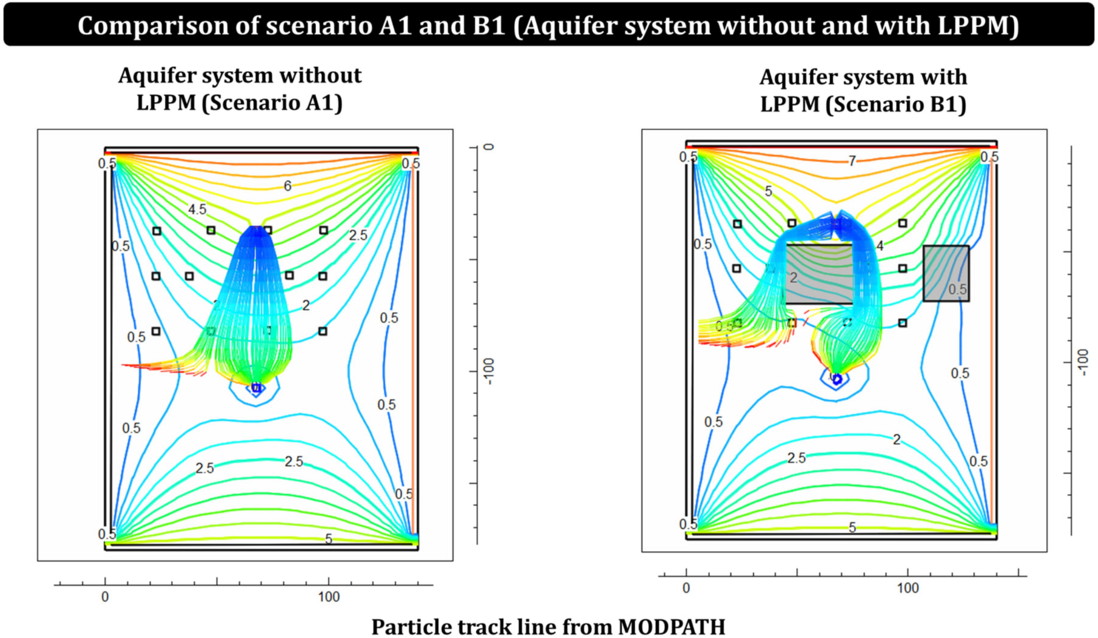


Figure 7: Particle track line predicted via MODPATH for aquifer system without and with LPPM

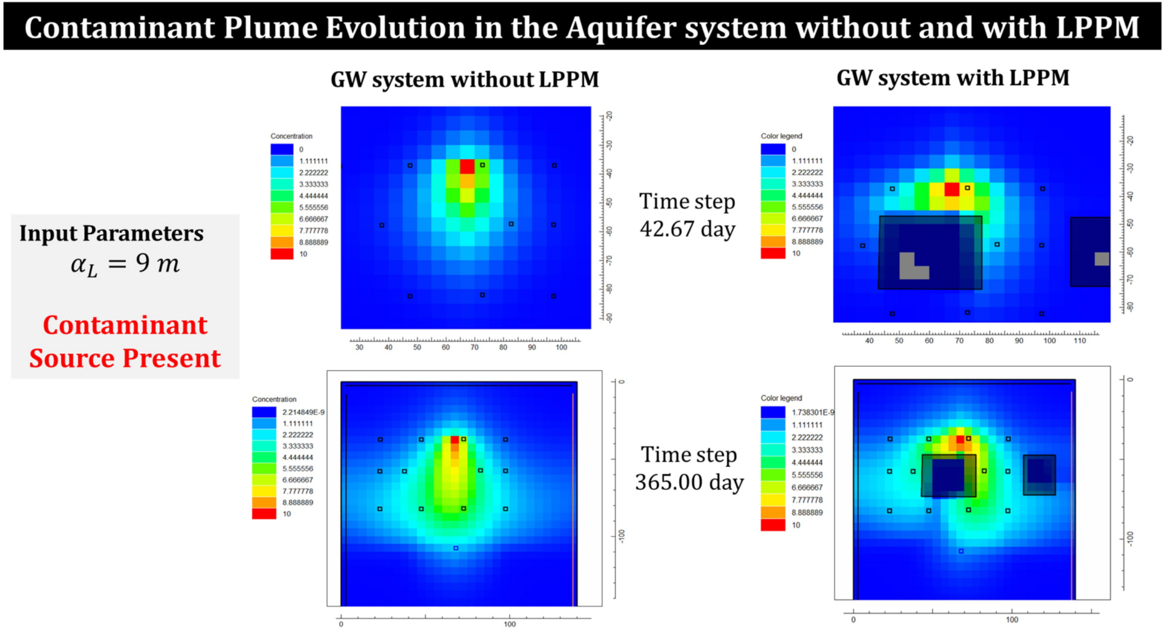


Figure 8 (a): Contaminant plume evolution for aquifer system without and with LPPM during loading period

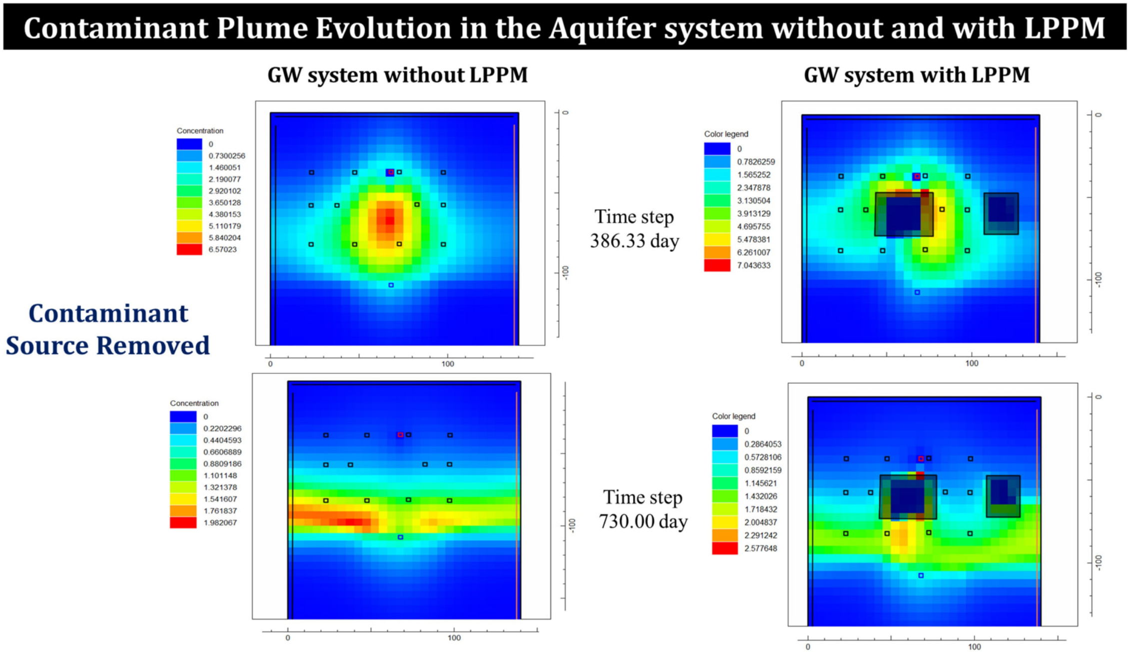


Figure 8 (b): Contaminant plume evolution for aquifer system without and with LPPM after source removal/isolation

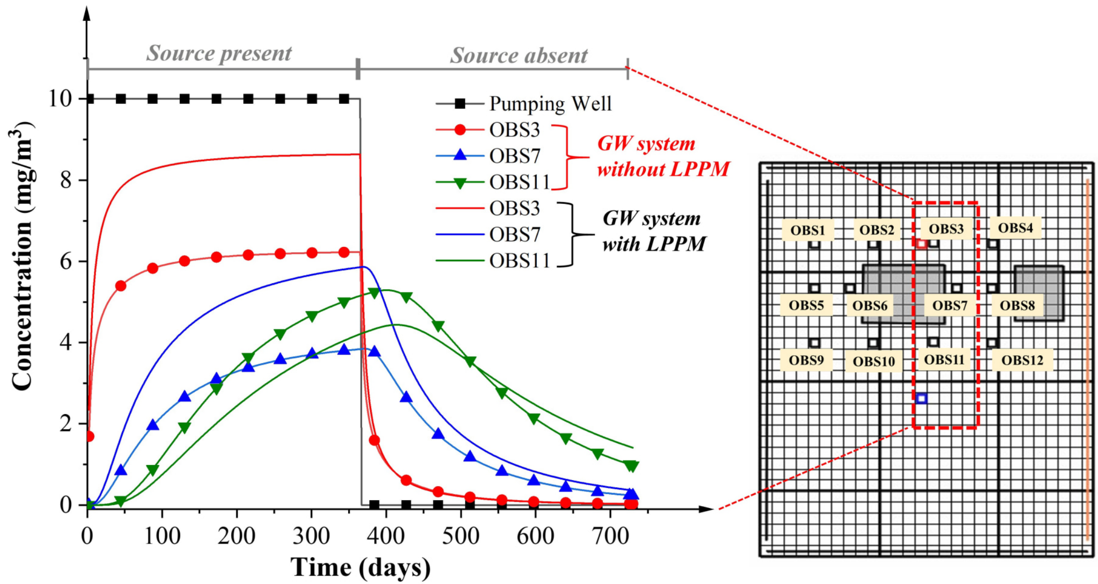


Figure 9: Comparison of BTC without and with LPPM

## (III) Effect of dispersion parameters on the contaminant transport behavior

### BTC at observation well 7

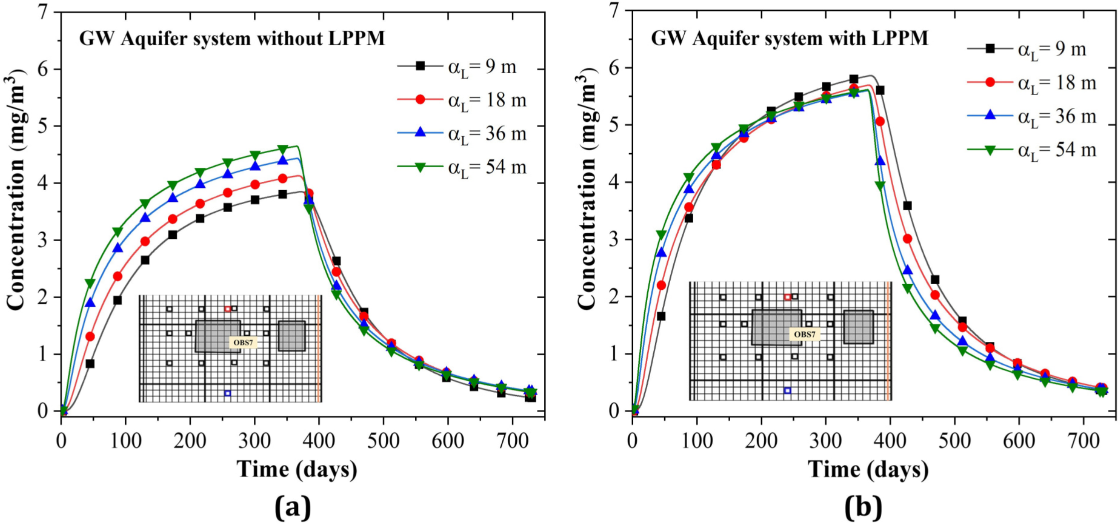


Figure 10: BTC predicted at observation well number 7 in the (a) absence and (b) presence of LPPM for different values of longitudinal dispersivity

- An early breakthrough was observed for $\alpha_L$= 54 m as compared to $\alpha_L$= 9 m for homogeneous aquifer systems, clearly depicting the effect of longitudinal dispersivity on BTC.

- The effects of dispersivity on the rising and falling limbs of the BTC were negligible for aquifer systems with LPPM.
- The impact of LPPM and longitudinal dispersivity on the peak concentration value was indistinguishable.

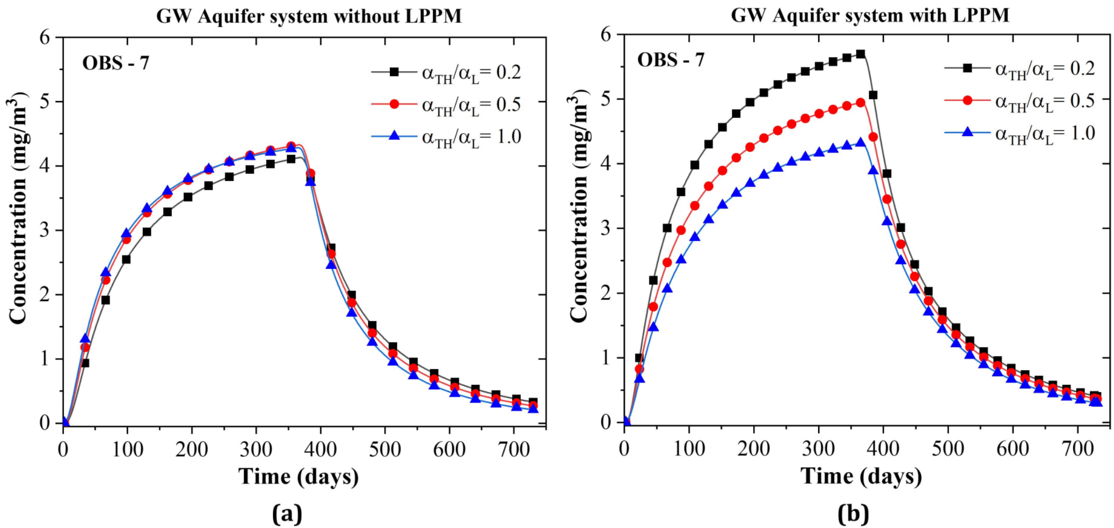


Figure 11: BTC predicted in the (a) absence and (b) presence of LPPM for different values of the ratio of transverse to longitudinal dispersivity

# DISCUSSION AND CONCLUSION

## *Discussion*

- During the source loading period, a very low value of the concentration of order $10^{-9}$ $mg/m^3$ was observed in the LPPM region.
- The spatial distribution of contaminant plume for aquifer systems with LPPM varied largely as compared to a homogeneous system.
- The maximum value of concentration in the aquifer with LPPM was found to be ~40% higher than the homogeneous system after source removal.
- After source removal, the maximum value of 1.98 $mg/m^3$ was observed for the homogeneous system at a location away from pumping and extraction well after 730 days; however, for a heterogeneous system with LPPM, the maximum value of 2.57 $mg/m^3$was observed.

## *Conclusion*

The numerical simulations carried out in this study mimic the realistic field-scale conditions and highlight the relevance of LPPM and associated transport processes on contaminant transport dynamics, which was usually overlooked.

# ABSTRACT

In this study, contaminant transport behaviour in the aquifer system (140 m × 180 m × 5 m) was analyzed using a 3-D groundwater flow and contaminant transport model viz. MODFLOW2005 and MT3DMS. The impacts of hydrodynamic dispersion parameters on the conservative contaminant plume dynamics were analyzed for homogeneous and heterogeneous aquifer systems with low permeability porous media (LPPM). The spatio-temporal distribution of contaminant concentration and breakthrough curves (BTCs) at 12 observation wells were used to analyze the transport dynamics due to conservative contaminant released from a single point source over a hypothetical study area for a period of 1 year (365 days). Results from MODPATH show a significant variation in the pathway of groundwater for homogeneous and heterogeneous aquifer systems. During the source loading period, a very low value of concentration of order $10^{-9}$ mg/m$^3$ was observed in the LPPM region. The spatial distribution of contaminant plume for aquifer system with LPPM varied largely as compared to homogeneous aquifer system. The maximum value of concentration in the aquifer with LPPM was found to be ~40% higher than the homogeneous system after source removal. After the source removal, the maximum value of 1.98 mg/m$^3$ was observed for the homogeneous system at a location away from pumping and extraction well after 730 days; however, for a heterogeneous system with LPPM, the maximum value of 2.57 mg/m$^3$ was observed. An early breakthrough was observed for $\alpha_L$= 54 m as compared to $\alpha_L$= 9 m for homogeneous aquifer system, clearly depicting the effect of longitudinal dispersivity on BTC. However, effects of dispersivity on the rising and falling limbs of the BTC were negligible for heterogeneous aquifer system with LPPM. Further, an impact of LPPM and longitudinal dispersivity on the peak concentration value at observation well (OBS-7) was undistinguishable. The numerical simulations carried out in this study mimic the realistic heterogeneous aquifer conditions and highlighted the relevance of LPPM and associated transport processes on contaminant transport dynamics at field-scale, which was usually overlooked.

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