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Modelling the dispersion of pollutants in porous underground environments.

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ATTESTATION DE CORRECTION DE LA THESE DE DOCTORAT/Ph.D

Nous, Professeur **MBINACK Clément**, Examinateur, et Professeur **TCHAWOUA Clément**, Président du Jury de la Thèse de Doctorat/Ph.D de Monsieur **MADIE YONTI Calvia**, Matricule **12W1316**, préparée sous la direction du Professeur **TOGUE KAMGA Fulbert** et sous la supervision du Professeur **WOAFO Paul**, intitulée : «**Modelling the dispersion of pollutants in porous underground environments**», soutenue le **Mercredi, 14 Juin 2023**, en vue de l'obtention du grade de Docteur/Ph.D en Physique, **spécialité Physique de l'Environnement Terrestre, option Sciences de l'Atmosphère,** attestons que toutes les corrections demandées par le Jury de soutenance ont été effectuées.

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Dedication

I dedicate this thesis:

- To **God Almighty** for all the strength and mercy, you give me everyday.
- To my wife **MADIE DJUIFOUO Marie Laure** .
- and my son **DEMANOU Christ Mercy Elisha**

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Abstract

The classical and fractional dispersion advection equation with distance and time-dependent dispersion and adsorption coefficients has been solved numerically. The finite difference scheme, the Runge Kutta 4 algorithm, and the implicit Euler method, based on a Grunwald and Caputo-Liousville approximation, were used to solve the models to explicitly evaluate the transport mechanism of contaminants in underground environments. The results suggest that the concentration profiles remain very sensitive to the distance-dependent dispersion coefficient. Furthermore, considering 0.1g/L of pollutant concentration as a guide value in the aquifer and considering a sinusoidally and exponentially time-varying initial pollutant source, the service time of a drinking water point is prolonged when the dispersion coefficient is distance-dependent and the adsorption coefficient constant. Two time-dependent dispersion functions were implemented to analyze the spatiotemporal variation in the domain. The results showed for values of k_L and k_A <1.2 years, significant solute mass retention is observed when the dispersion function is asymptotic. The concentration profiles are similar when values of k_L and k_A ≤ 1.2 years. Better solute mass retention was observed for the fractional advection-dispersion (FADE) model compared to the classical advection-dispersion(ADE) model. On the other hand, the absorption parameter (k_d) of the retardation coefficient has a significant impact on the dispersion of pollutants in subsurface media compared to the sorption intensity (n). This study highlights the need to update the transport parameters while modeling solute transport in porous media.

Keys words: Groundwater, Contaminant transport, drilling, human health, fractional-advection-dispersion.

Résumé

L'équation d'advection dispersion classique et fractionnaire dont le coefficient de dispersion et d'adsorption dépendent de la distance et du temps a été résolue numériquement. Le schéma de différences finies, l'algorithme de Runge Kutta d'ordre 4 et la méthode d'Euler implicite, basée sur une approximation de Grunwald et Caputo-Liousville ont servi à la résolution des modèles pour évaluer explicitement le mécanisme de transport des contaminants dans des milieux souterrains. Les résultats suggèrent que, les profils de concentration restent très sensibles au coefficient de dispersion dépendant de la distance. De plus en considérant 0.1g/L de la concentration des polluants comme valeur guide dans l'aquifère et en considérant une source initiale de polluant variable sinusoïdalement et exponentiellement en fonction du temps, le temps de service d'un point d'eau potable se prolonge lorsque le coefficient de dispersion est dépendant de la distance et le coefficient d'adsorption constant. Deux fonctions de dispersion dépendant du temps ont été mises en oeuvre pour analyser la variation spatio-temporelle dans le domaine. Les résultats ont montré pour les valeurs de k_L et k_A<1.2 ans, une rétention importante de la masse de soluté , observée lorsque la fonction de dispersion est asymptotique. les profils de concentrations sont similaires lorsque les valeurs de k_L et $k_A \leq 1.2$ ans. Une meilleure rétention de la masse des solutés a été observée pour le modèle d'advection-dispersion fractionnaire (FADE) par rapport au modèle d'advection-dispersion classique(ADE). D'autre part, le paramètre d'absorption (k_d) du coefficient de retard a un impact important sur la dispersion des polluants dans les milieux souterrains par rapport l'intensité de sorption (n). Cette étude met en évidence la nécessité de mettre à jour les paramètres de transport tout en modélisant le transport de soluté en milieu poreux.

Mots clés : Transport contaminant, forage, santé humaine, advection-dispersion fractionnaire

List of symbols

c : Solute concentration $[ML^{-3}]$

c_0: Source concentration, $[ML^{-3}]$

x: Observation thickness, [L]

t: Time variable[T]

R= retardation factor

$R(x)$=Depth-dependent retardation factor

Φ: Soil porosity

$D(x)$: Depth-dependent dispersion coefficient $[L^2T^{-1}]$

D_O : Molecular diffusion coefficient, $[L^2T^{-1}]$

α:Asymptotic dispersivity constant, $[L^2T^{-1}]$

$\alpha(x)$:depth-dependent asymptotic dispersivity, $[L^2T^{-1}]$

a: Asymptotic dispersivity constant, [L]

b: Characteristic distance, [L]

x_0: Transition zone , [L]

v : Fluid flow velocity,$[LT^{-1}]$

$K(x)$: Depth-dependent adsorption coefficient, $[L^3M^-1]$

K_d: adsorption coefficient, $[L^3M^-1]$

K_0: Adsorption coefficient in the topsoil, $[L^3M^-1]$

w: Frequency, $[T^-1]$

λ :Decay rate constant, $[T^-1]$

L : Length of the finite spatial domain, [L]

ρ_s : Soil density , $[ML^{-3}]$

$t_{1/2}$:Half-life time , [T]

$\Delta(x), \Delta(t)$, : Spatial and temporal steps , [L, T]

General introduction

Transport of dissolved contaminants by heterogeneous hydrogeology relies on expressions of their functional parameters. Solute transport in subsurface media remains of great interest in subsurface hydrology today [1]. The problem of solute dispersion during fluid movement in underground media was the focus of interest at the beginning of this century. That the general topic of hydrodynamic dispersion or miscible displacement became one of the most systematic studies [2, 3]. Decontamination of groundwater, when possible requires techniques and costs that are often unaffordable, and the abandonment of the exploitation of this (polluted) water then leads to severe economic and social consequences. In most African countries, including some large areas of Cameroon (far north), more than half of the population relies on groundwater, which is also an important source for agriculture, and industry. While the abundance of groundwater is an immutable reality, its distribution is rather complex. Careful studies are needed for the detection and characterization (qualitative and quantitative) in groundwater environments.

Advection-dispersion equation modeling to simulate groundwater flow processes and transport is essential for better management of these resources that have significant social and economic [4] . Advection -dispersion equation models allow rapid localization of water potability sites in groundwater environments. The mathematical statement of the solute transport equation, also called the advection-dispersion equation, has been accepted as a model to describe the migration and position of solutes in groundwater [1, 3]. The advection-dispersion equation (ADE) is assumed to be the most widely used method nowadays to model the transport of contaminants in subsurface environments. It describes contaminant transport processes in homogeneous porous media. However, it becomes less efficient to adequately capture this in heterogeneous porous media [5, 6] . Because ADE is based on the assumption of Fick's first law, while the solute transport process in heterogeneous porous media is in accord with a non-Fickian or anomalous mechanism [5]. Non-local transport models are alternative models proposed to explain the nonfiction transport process. These models generate the spatial fractional advection-dispersion equation (s-FADE) and the temporal fractional advection-dispersion equation (t-FADE). FADEs have been successfully applied to simulate solute transport in homogeneous and heterogeneous, saturated and unsaturated soils at the laboratory scale [22], in a sand and gravel aquifer , and a highly heterogeneous aquifer . Many works [1, 2, 4, 7–13] have been carried out by uniting ADE and FADE models to determine and locate the level of contamination in subsurface environments, they have nevertheless shown considerable weaknesses.

An analytical solution of the contaminant transport equation in soils with depth-dependent delay coefficients and time-dependent input boundary conditions was developed by [1, 4] by evaluating the effects of depth-dependent delays on the fate and transport behavior of the contaminant in a porous medium. These authors neglected the impact of the asymptotic depth-dependent dispersion coefficient in the aquifer as formulated by [14] Sharma, 2015. In a heterogeneous medium, the pollutant transport equation considering a constant dispersion coefficient becomes irrational for predicting contaminant retention in aquifers. Field and experimental evidence from studies have been suggested by [15–19] that the dispersion coefficient is not constant but increases with time displacement or equivalently with solute travel distance. The apparent increase in the coefficient of dispersion has been called the scaling effect by [10]. The scaling effect is generally attributed to the heterogeneity of the pore formation, particularly in the heterogeneity of the hydraulic conductivity. Stochastic analyses have shown that dispersivity depends on travel time and increases until it reaches an asymptotic value [20], and the theoretical deterministic analysis of [4] has also established that dispersivity in a stratified aquifer is time dependent. Therefore, there is ample evidence that the scale of the dependence causes the dispersion to vary in time and space. A semi-analytical solution of the transport model with distance-dependent asymptotic dispersivity was developed by [14] with a constant pollutant source at the aquifer inlet and constant asymptotic dispersivity parameters in a heterogeneous porous medium. This author neglected the variability of asymptotic dispersivity parameters in a heterogeneous porous medium. A numerical solution of the Burgers equation obtained by the unconditionally stable Crank-Nicolson finite difference scheme was developed by [2] to analyze the constant and longitudinal dispersion profile of contaminants. These studies did not consider the variation in time- and space-dependent dispersion coefficients, decay rate constant and zero-order solute production rate coefficient in the liquid phase as done by the work of [21] with a linear dispersion advection equation model.

A mathematical model with four types of input conditions, namely, continuous constant, pulsation, exponential decay, and sinusoidal variation was developed by [13] to evaluate the variability of dispersion coefficient on temporal and spatial scales on the transport mechanism of contaminants in saturated porous media subjected to nonlinear sorption model. [13] developed an advection-dispersion equation (ADE) model that remains to this day less successful in adequately capturing pollutants in heterogeneous porous media than [6]. Moreover, it did not take into account the variability of sorption parameters of the Freundlich model on pollutant dispersion in aquifers. Similarly, [22]does not allude to the adsorption coefficients (Kd) and absorption intensity (n) in their work, these parameters play the role of causing a delay of solute concerning the mobile fluid in fractured rock. [22] memorized an experimental study associated with the model (s-FADE) to model the conservative solutes, where their results show that the best simulation was obtained from the s-FADE model compared to the ADE model.

The mechanisms of transfer, dispersion, or transport of contaminants in groundwater are very complex due to the highly heterogeneous nature of porous media. The contamination of groundwater by pollutants, which remains the biggest problem for the health of the world's inhabitants and agriculture, is the central theme of this thesis. Given the poor quality of water in aquifers and the consequent high cost of treatment, this work aims to determine the location of groundwater sources in the world. This work aims to determine the location of drinking water points and their consumption times in relation to the source of the pollutants, by evaluating the effect of dispersion and adsorption models of contaminants on the spatio-temporal distribution of pollutants in a porous medium in a groundwater table of finite thickness. Efforts are made by the scientific community to overcome this problem, in this same context, to make our contribution to the understanding of the fate of pollutants introduced into the groundwater environment. So the specific objectives of this work are:

- Provide a numerical solution of the transport equation by associating the asymptotic dispersive and reaction function that is a function of the aquifer thickness, with three profiles of initial pollutant concentration conditions (constant (a), exponentially(b), and sinusoidally(c) variable as a function of time, imposed at the aquifer inlet to evaluate the pollutant concentration profile in the subsurface media.

- Numerically solve the Burgers equation associated with longitudinal dispersion phenomena as a function of time, to discuss and determine the dispersion parameters related to the concentration profiles using the two time-dependent dispersion coefficients.

- To study the concentration profile of the pollutants as a function of the parameters n (sorption intensity or Freundlich parameter) and the adsorption coefficient (Kd) on four points taken in the aquifer to select the n values and the adsorption coefficient (Kd) at the exit of the aquifer using two models (ADE) and (FADE) to optimize the retention of the pollutants in the groundwater environment

  This work is mainly composed of three chapters and obviously of an introduction and a general conclusion while ending with some perspectives. Chapter 1 is dedicated to the literature review, basic notions on subsurface environments. In chapter 2, the different parameters and models used are presented as well as the different methods used to obtain the results. Chapter 3 presents, comments and discusses the main results obtained.

CHAPTER I

REVIEW AND BASIC PRINCIPLES OF SUBSURFACE POROUS MEDIA.

1.1 Introduction

Subsurface porous media are aquifers composed of discrete particles such as sand, aggregate, and gravel. Groundwater occupies the interstitial voids (pores) of the grains through which it flows [21]. The quality of water flowing through subsurface porous media depends on temperature and pressure conditions, the types of rocks and soils through which it flows, and residence time. In general, when pores are large, water flows faster and dissolves less material. Groundwater flowing through an aquifer is naturally filtered, and this filtration, combined with a long subsurface residence time, is evidence that groundwater contains less undissolved material than surface water [23,24,25] . This chapter aims to give a non-exhaustive history of the modeling and dispersion of pollutants in groundwater environments. We will first present the generalities and a brief history of subsurface environments. The second part will be dedicated to the presentation of the mechanism of transport of pollutants and some mathematical models to describe the flow of fluids in underground environments. At the end, we will make a brief reminder on the numerical methods of resolution.

1.2 General information on underground environments.

environments are a step in the transit cycle of waters containing them to the oceans and seas. The nature of the subsurface conditions is the extent and duration of contaminant transits in subsurface environments [21]. This results in a typology of aquifer systems that are, on either side of the threshold of the subsurface environments, continuous with the surface water system. Rainwater infiltrated into the subsurface, during an effective rainfall, and flows through the various pores and microcracks in the aquifer rocks, these aquifers are composed of two parts [22]. The unsaturated zone consists of the soil and the upper part of the aquifer rock. In this zone, the entire pore space of the rock is not completely saturated with water. Subjected to both the forces of capillarity, which has the role of drawing water upward to the top layer of soil acting as a blotter, and gravity, which draws it downward, the water in the unsaturated zone is in constant motion [26] . Some of it eventually moves downward and wets deeper and deeper layers, until it reaches an impermeable layer. Above this impermeable level begins the saturated zone where water flows through every gap in the rock and into every possible void. The water flows underground over the impermeable layer, most often following the topography, sometimes for tens or even hundreds of kilometers [12]. Groundwater can emerge in the open air, on the surface of the ground, forming a spring at the origin of a watercourse, in areas topographically lower than their recharge area. In this case of the aquifer, with an unsaturated zone and a saturated zone, the roof of the water table is at atmospheric pressure and we speak of a free water table. The water table can rise or fall with precipitation, in the form of seasonal and annual fluctuations [22]. When water from a water table flows into the subsurface, it can become pressurized under an impermeable layer. This is referred to as a confined aquifer, which is usually deep, a few hundred meters and more [56]. The water in it is mostly under pressure and when it is released by a borehole, which penetrates the impermeable layer, it can gush to the surface naturally: such an aquifer is then called artesian. When the rocks are too fractured, they form an aquifer, and wells can be drilled to draw groundwater [27]. Most groundwater is concentrated in the pores of the rock, but these are very poorly connected, not allowing for efficient water flow. The rock fractures, on the other hand, include less water but allow sufficient groundwater flow for capture [21].

Water containing pollutants, such as sewage and radioactive waste, infiltrates the soil matrix, as does direct runoff from surface areas. This water eventually enters the aquifer and, under the influence of distance and soil parameters, becomes a source of drinking water. During the passage of water through the soil, pollutants are mixed, adsorbed, dispersed, and diffused in the flow. The classical porous domain considered for the present study is shown in Figure 1 below by [28].

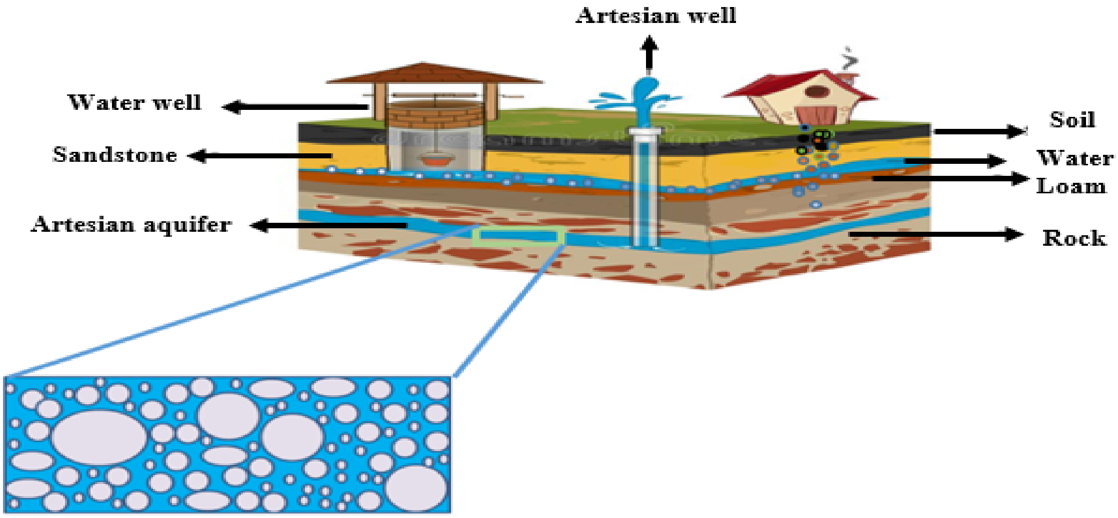

Figure 1.1: Representation of a porous medium, each bubble representing the interstitial spaces.

1.2.1 Brief history of underground environments studies

the geological history of a subsurface environment provides information about the nature and arrangement of the different geological materials within it. This information is critical to understanding groundwater flow and is a good clue to locating the best aquifers [26, 29]. Pumping tests were conducted by [30] on a basaltic groundwater aquifer of Tertiary and Quaternary age in the Snake River Plain, Idaho, northwestern United States. They conclude that the aquifer consists of a thick sequence of several flows, interbedded with sedimentary horizons. A packer system was installed in the wells and boreholes to isolate specific intervals of the aquifer and perform pumping tests.

1.2.2 Main types of aquifers containing the groundwater environment

aquifer is a set of permeable rocks with the property to store groundwater and ensure its flow to a source [22, 31] . It consists of a saturated zone (solid medium + water) and an unsaturated zone below:

An unsaturated zone: water does not fill the pores and is translated into the permanent movement towards the surface, and towards the depths.

A saturated zone: Water fills all the pores and flows into the subsoil over the impermeable layer, following the topography over several tens or even hundreds of kilometers. Groundwater can resurface at the surface of the ground, giving rise to a spring that is the origin of a stream [30]. There are three major families of aquifers that constitute groundwater reservoirs:

- Sedimentary aquifers are composed of limestone, sand, sandstone, and chalk. They characterize the large Aquitaine basins.
- Alluvial aquifers are made up of fine silts deposited by rivers during floods, and floods, interspersed with sands and gravels.
- Alluvial aquifers are made up of fine silts deposited by rivers during floods, intercalated with sands and gravels. during floods, interspersed with sands and gravels [32].
- Aquifers of crystalline rocks, granite, and volcanic keep water in cracks and altered areas. They shelter small water tables and are frequent in the Alps, the Massif Central, and the Pyrenees [31]. The two properties of the aquifer, porosity, and permeability, allow us to break down the different associates into three types:
- Porous, the limestone rocks are very porous and suitable for dissolution by water
- Karstic, Limestone plateaus, where the voids are mostly cracks that can be the size of chasms and caves (karst), contain some water tables.
- Fissured, crystalline rocks have very little porosity. The water is contained and circulates in the faults or cracks of the rock.

1.2.3 Groundwater

Groundwater remains one of the best sources of drinking water for the population in most regions of the world [33]. This resource is the basis of a country's economy and must be managed sustainably, consistently and rationally because it is threatened by various sources of pollution of geogenic and anthropogenic origin. Groundwater acquires its chemical composition mainly according to the geological nature of the environments crossed, the residence time in the reservoir and the reactive substances that it may encounter during the flow [23]. The chemical composition of groundwater can be altered by undesirable or toxic substances from livestock, agricultural activities (nitrates, ammonium, pesticides, fecal organisms), industrial (heavy metals, phenols, cyanides, trichloroethylene, tetrachloroethylene), human (nitrates, fecal organisms, synthetic trace hydrocarbons) and the surrounding rock, especially of saline origin, which makes these waters unsuitable for consumption. Water plays the role of regeneration of new cells and organs in human beings. But it contains pollutants and remains the vector of transmission of several diseases [34]. In many African countries, particularly in Cameroon, the far north region and others, the supply of drinking water to rural populations is provided by wells and boreholes. Most of these structures, apart from a few physicochemical analyses carried out to ensure the potability of water after the creation of a borehole and before delivery to the population, do not undergo any quality control on a regular basis [24]. The intensive and uncontrolled use of agricultural inputs and leakages during the rainy season have a negative influence on the quality of these waters.

1.2.4 The water cycle - Origin of groundwater

Water occupies three-quarters of the surface of our planet. It is known for rivers, groundwater, lakes, seas, and oceans. It is concentrated in soils and gathers all kinds of living beings, water contributes to the water cycle. Water plays a fundamental role in most of the physicochemical processes that affect the earth's crust; together. Rivers and underground aquifers play a crucial role in this system. The water cycle is the permanent exchange of water between the seas and oceans, surface and groundwater, the atmosphere, and the biosphere [35] . This exchange takes place in the atmosphere where water moves in the form of water vapor and on land where water circulates on the surface or underground. It is precipitation that feeds groundwater. On average, 65% of the precipitation that reaches the Earth evaporates, 24% runs off and 11% infiltrates. But only part of it is available for groundwater recharge, as the part is reserved by the soil and plants and part feeds lakes and rivers by runoff; only the balance slowly infiltrates into the soil and subsoil. Rainwater flows into the pores and cracks of the rocks; this is called reservoir rock or aquifer.

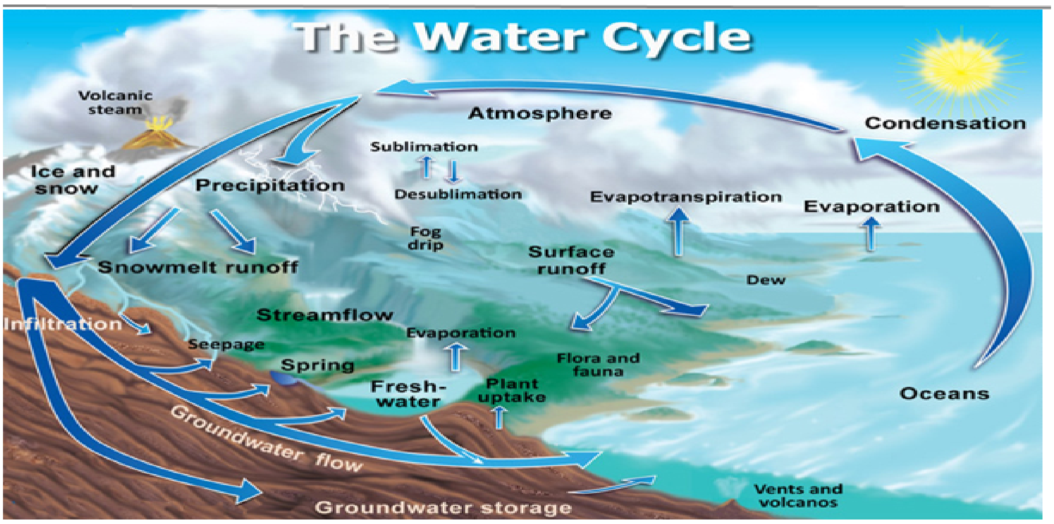

Figure 1.2: Water cycle (Science.nasa.gov, 2018)

1.2.5 Pollution and chemical composition of groundwater

Groundwater mineralizes to varying degrees due to soil/rock-water interactions, the latter leading to the dissolution of certain minerals and chemical elements [36]. Nine main chemical elements (Na, Ca, Mg, K, HCO3, Cl, SO4, NO3, Si) account for nearly99% of the solute content of natural groundwater. The dissolution density depends on the path distance, residence time, the solubility of soil/rock minerals, and the amount of freshwater dilution by recharge [37]. The reactions of rainwater in the soil/rock portion during infiltration provide groundwater with its mineral composition [38, 39] . Groundwater in recharge areas of humid regions is likely to have less considerable overall mineralization, compared to arid or semi-arid regions where the combination of concentration by evaporation and slower movement of groundwater, can produce much more considerable concentrations [40]. Water is the preferred vector for the dissolution, transport, and dispersion of pollutants in the deep subsoil. Agricultural spreading is often blamed for polluting the water table, as it creates over-fertilization. Excess nitrogen is washed away by rainfall in winter to pollute rivers or groundwater [41–43] . Diffuse pollution acts on large geographical areas. It mainly comes from unreasonable agricultural activity (use of fertilizers over crop needs [44, 45] . As the catchments are mainly located in rural areas, groundwater is exposed to the risk of contamination by pollutants of agricultural origin.

- **Nitrates**

  Often applied in excess to crops to improve yields, nitrogen fertilizers are not fully consumed by plants. They are transformed into highly soluble nitrates and transported by seepage water to groundwater [45, 46] . Since the percolation of nitrates into the subsurface requires significant time lags, aquifer contamination can only be observed decades later when effective curative action is no longer possible [42] . The only prevention is therefore possible to improve the situation [41] . But already, with the continuous increase of nitrate concentrations in the main aquifers of the basin, pollution by nitrogen compounds is becoming more and more worrying. Some waters exceed the admissible threshold of potability set at 50 mg/l and sometimes exceed levels above 100 mg/l [47]. These levels are downgrading parameters that force the abandonment of catchment sites. Current projections show that within 30 to 60 years, with identical farming practices, the maximum allowable concentrations of nitrates in groundwater will be largely exceeded (50 mg/l). The challenge is to react quickly before the nitrate front spreads to all aquifers and to engage in further research to better understand their toxicity [39, 48].

- **Pesticides** Pesticide pollution is mainly related to agricultural activity where plant protection products are used to control any pest or crop-competing species. In addition, the self-purifying power of the soil generally destroys the molecules during their migration to the aquifer [36]. The levels recorded in the regional aquifers are thus below the thresholds set by the drinking water quality standards. In addition, each year, new chemicals are marketed, increasing the diversity of molecules used and imposing the need to strengthen research efforts and knowledge of their effects [49].

- **Dissolved mineral salts**

  Groundwater can naturally contain sulfates and chlorides as a result of the dissolution of naquifer rocks. But their content sometimes increases considerably following industrial discharges, and infiltration of chemical fertilizers. These pollutions are mainly encountered in large industrial and urbanized areas [38] .

1.2.6 Physico-chemical characteristics of transport in the groundwater environment

Dissolved solutes in groundwater are responsible for several physicochemical processes. In addition, simple migration processes can be adsorbed onto mineral grains in the aquifer, and participate in oxidation-reduction reactions, which biodegrade or even disappear from the solution [39]. As a result of sorption processes, to have, some solutes advance through the aquifer much slower than the flow of water that carries them. In contrast, radioactive decay, biodegradation, and precipitation will cause a decrease in concentration but will not slow the rate of movement [42]. Finally, there may be times when the velocity of the element is faster. During their movement, pollutants can influence three kinds of phenomena:

- Delay which is an immobilization, often reversible (sorption, ion exchange, filtration, precipitation)
- Attenuation is an irreversible disappearance or transformation (chemical oxidation-reduction, biological oxidation-reduction, biodegradation, volatilization, hydrolysis)
- Increase in mobility: accelerated speed (dissolution, ionization, complexation, chelation)

1.3 Transport mechanisms of pollutants in underground environments.

Chemical transport in subsurface media is affected by a large number of processes and properties of porous media, such as convective transport with flowing water, molecular diffusion, hydrodynamic dispersion, equilibrium or non-equilibrium exchange with the solid phase, reactive solutes involved, and possibly production and decay processes [3, 50] . The movement of the pollutant in a subsurface environment is the result of two major terms, firstly advection so the process involves each molecule of a non-reactive solute moving at the average speed of water movement. The second component is dispersion, which tends to propagate the molecules along the direction of flow in the subsurface medium [51].

1.3.1 Transport by advection

Advection is the component of solute movement attributed to average groundwater flow. In other words, it is the transport of the dissolved contaminant at the average pore velocity of the fluid in the medium. Advective transport is the movement of the solute under the action of the motion of the water in which it is dissolved [50]. To consider advective transport alone is to consider that each solute molecule moves at the speed of the elementary volume of water that contains that molecule. The basic driver of pollutant transfer in solution in aquifers is that which governs the movement of the entire liquid phase; this is the gravity field [52]. This mechanism is called "advection" or sometimes "convection". The advective transport of pollutants can be described in mathematical terms as follows

$$\frac{\partial c}{\partial t} = -v_{0x}\frac{\partial c}{\partial x} \tag{1.1}$$

This equation is the analog of Darcy's law for the evolution of the concentration under the effect of The water movement, v_{0x} is Darcy velocity of groundwater flow.

1.3.2 Dispersion

The role of dispersion is to describe the spread of pollutants in the natural environment. Dispersion is a phenomenon that results in the distribution of the pollutant's travel time around the average transfer time. Indeed, some molecules move faster and others slower than the average speed of water [52]. The dispersion coefficient is therefore a crucial parameter, especially for pollution risk assessment, since dispersion dilutes concentrations but also spreads the arrival times at a point [21]. Dispersion depends on two processes: hydrodynamic dispersion and molecular diffusion.

Hydrodynamic dispersion

The hydrodynamic dispersion derives from the microscopic scale of the distribution of velocities inside the pores caused by friction on the walls, the difference in the size of the pores along the path followed by the molecules, and the tortuosity (ratio between the distance that would be traveled in a straight line by a particle and the distance traveled through the pores) of this path Figure (1.3). The hydrodynamic dispersion phenomenon also involves diffusion kinematic (mechanical) dispersion [3,52]. Due to the microstructure of the medium, the fluid velocity varies in magnitude, and direction within the porous medium. This variation in velocities results in dilution of the pollutant, kinematic dispersion.

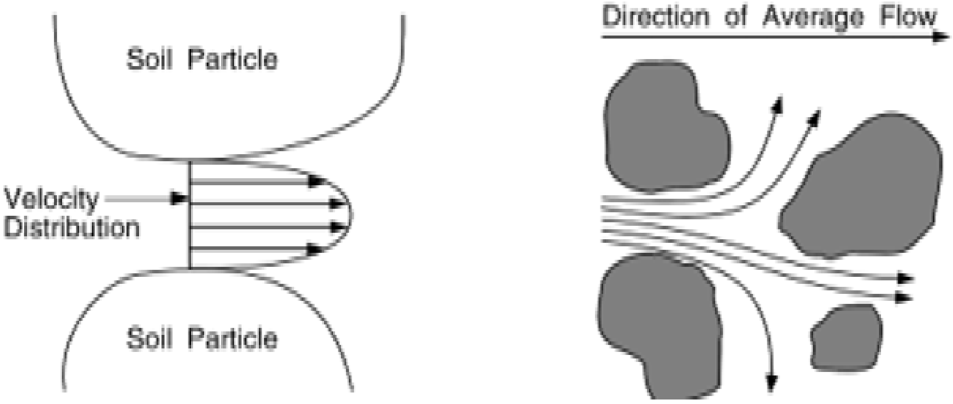

Figure 1.3: hydrodynamic dispersion phenomenon

Molecular dispersion

Molecular diffusion is a Brownian phenomenon (random movement of the molecules) which causes the displacement of the solute of a region with high concentration towards a region of lower concentration figure 1.4.

Molecular diffusion can occur independently of advection; it is a physical phenomenon related to molecular agitation [53]. This process at the macroscopic scale can become an important transport mechanism if the flow velocities are very slow. However, it is generally negligible compared to hydrodynamic dispersion in aquifers [52]. If there is

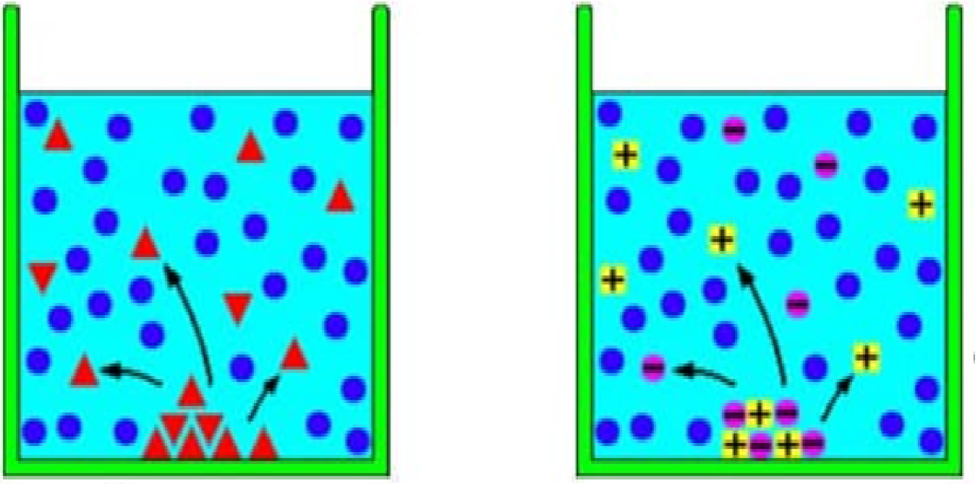

Figure 1.4: Molecular diffusion phenomenon

a concentration gradient between two neighboring points, the more concentrated one will see on average more particles in all directions than the less concentrated one. The result will be a transfer of particles from the more to the less concentrated areas, according to the classical Fick's law where the molecular diffusion coefficient translates the proportionality of the mass flow to the concentration gradient . The mathematical writing of the molecular diffusion coefficient is:

$$D^* = \frac{D_{mol}}{\tau} \tag{1.2}$$

Where D_{mol} is the molecular diffusion coefficient of the pollutant in water in the absence of solid, τ is the tortuosity of the medium.

1.3.3 Dispersion with a variable coefficient depending on time and thickness of the subsurface medium

A detailed study of the effect of scale on dispersion in the field is conducted by [18] who suggest that the dispersivity associated with the dispersion coefficient is not constant but rather depends on the average distance traveled by the solute in the porous medium Figure 1.5. The dispersivity parameter is a measure of the dispersive properties of a system, a traditionally is considered a single-valued characteristic property of the entire medium [28, 52, 54] .

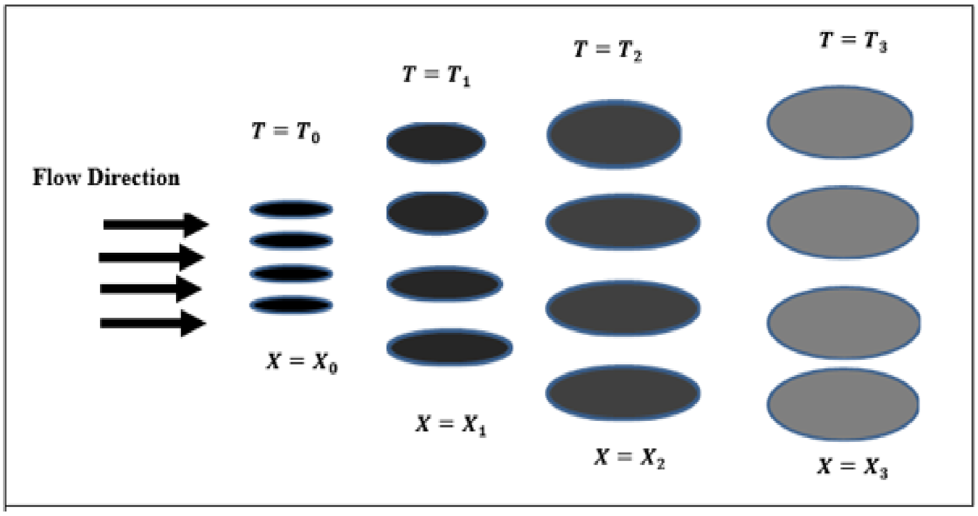

Figure 1.5: Dispersivity phenomena are distance and time dependent

The dispersivity is the function of the average distance traveled to bring out an equation relating the diffusion coefficient of particles suspended in a fluid to the variance of the distribution of particles in a time interval. Assuming that mechanical dispersion is analogous to diffusion, i.e. Fickian, this equation was used by [55] in studies of dispersion of a solute during the transport of a moving fluid in a porous medium. The equation is written:

$$D = \frac{1}{2}\frac{d\sigma^2}{d\bar{x}} \tag{1.3}$$

Where D is the dispersion coefficient, σ is the spatial variance of the tracer or solute distribution, and t is time.

The relationship (1.3) shows that the distribution will increase linearly with time (or mean distance displacement) when the dispersion coefficient is constant. For hydrogeological situations where the contribution of diffusion can be considered negligible compared to mechanical dispersion, D in (1.3) represents the mechanical dispersion coefficient. Assuming that the mechanical dispersion is equal to the product of the dispersivity and the average pore water velocity [54]and recalling that is equal to the distance traveled by the solute in time t, an expression for the dispersivity can be derived from (1.3) can be written :

$$\alpha = \frac{1}{2}\frac{d\sigma^2}{d\bar{x}} \tag{1.4}$$

Where α is the dispersivity and is the average travel distance. [56] used (1.2) to obtain values of the dispersivity factor from laboratory tracer tests. Since the average displacement distance is directly proportional to elapsed time, the dispersivity also varies with time. When dispersivity is scale-dependent due to environmental heterogeneity, several complex functions are needed to describe dispersivity [25, 52] . The functions can be either spatial or temporal. When these functions are used in place of the dispersion constant in the ADE, the resulting models are commonly called scale-dependent CDE models. Such models would include both the distance and time dependent ADE categories as they have been used to describe dispersion [57]. The scale-dependent dispersivity functions (noted as linear, parabolic, asymptotic, and exponential) are presented below:

- **Distance-dependent dispersivity** The linear distance-dependent dispersivity function below :

  $$\alpha = E\left(1 - \exp(-F\bar{x})\right) \tag{1.5}$$

  This form has for application, the analytical solutions of a concentration with zero or constant boundary condition for a constant flux. [18]have also proposed the distance dependent dispersivity function in four forms:

  ?Linear form

  $$\alpha(x) = a\bar{x} \tag{1.6}$$

  Parabolic form

  $$\alpha(x) = a\bar{x}^{b} \tag{1.7}$$

  Asymptotic form

  $$\alpha(\bar{x}) = a\left(1 - \frac{b}{\bar{x} + b}\right) \tag{1.8}$$

  Exponential Form

$$\alpha = E\left(1 - \exp(-F\bar{x})\right) \tag{1.9}$$

Where $\bar{x}$ is the average distance traveled, b and F are constants, a and E are asymptotic or maximum value of dispersivity, b is characteristic half-length (equivalent to the average distance travelled corresponding to a/2). These four forms have the application, firstly to fit the dispersivity equations to compare the variances of the tracer distribution with the finite elements to obtain the results of the model [58]. Subsequently, the scale-dependent dispersivity is necessary for the prediction of pollutant transport for short-distance paths, however, the scale-dependent early dispersivity.

- **Time-dependent dispersivity**

  [58] proposed the time-dependent dispersion function in three forms: Linear form

Linear form

$$D(t) = D_0\frac{t}{t+k} + D_m \tag{1.10}$$

Asymptotic form

$$D(t) = D_0\left(1 - \exp(-t/k)\right) + D_m \tag{1.11}$$

Exponential form

$$D(t) = D_0\left(1 - \exp(-t/k)\right) + D_m \tag{1.12}$$

WhereD_0 is the maximum dispersivity, D_m is the molecular diffusion, and k is equal to the average travel time corresponding to $D_0 + D_m$ in the linear case, to $0.5D_0 + D_m$ in the asymptotic case, and $0.632D_0 + D_m$ for the exponential case [58] . The three forms of time-dependent dispersivity have for application, the transport of pollutants in an infinite medium, following the explicit analytical solution for the case of instantaneous injection in the end the analytical solution and numerical integral for the case of continuous injection.

1.4 The transport of reactive solutes in underground media

1.4.1 The adsorption coefficient linked to the delay coefficient

Transport of dissolved contaminants by heterogeneous hydrogeology relies on expressions of their functional parameters. The nonlinear uptake related to the lag coefficient is one such parameter inheriting significant ambiguities in its estimation when subjected to heterogeneous flow conditions [13]. This solute transport in subsurface environments remains of great interest to subsurface hydrology today [1]. The transport processes that govern the transport behavior of solutes in heterogeneous subsurface media are advection, dispersion, diffusion, sorption, and degradation. Among these processes, sorption and degradation play an important role in the decision of solute infiltration and distribution in the heterogeneous porous medium [59]. Several processes act simultaneously on the chemical constituents transported through the soil. This requires that quantitative descriptions of chemical transport include feasible processes such as the intensity of contaminant uptake into the subsurface environment. Predicting the concentration of pollutants in the soil matrix is very important to minimize the risk and vulnerability of aquifers [1]. In addition, the accuracy of the predicted model is crucial to adequately assess and predict the transport behavior of contaminants in the subsurface. Solute transport in groundwater systems is traditionally modeled by the classical advection-dispersion equation that can add up to an equilibrium uptake. The nonlinear sorption model at the unit fracture scale showed that below the pollutant concentration, the retardation factor increases with the Freundlich isothermal exponent n, while the reverse occurs above the same concentration [13, 60]. Due to hydrodynamic dispersion, the concentrations in the plume decrease towards the edges of the plume. The delay factor associated with nonlinear absorption is shown below:

$$R_d = 1 + \frac{\rho_b}{\theta} k_d n c^{n-1} \tag{1.13}$$

R_d is the adsorption coefficient and n is the sorption intensity. ρ_b is the specific weight of the solid particle in the matrix, θ is the porosity of the medium, n is the Freundlich exponent.

1.4.2 adsorption coefficient with Variable coefficient depending on the thickness of the underground medium

The physical (advection, diffusion, and dispersion processes) and reaction (adsorption and degradation) models control the transport of contaminants described in the numerical model [61]. Adsorption and degradation processes in soils are often related to the amount and type of organic matter and microbial activity strongly dependent on depth [10]. Soil organic matter content has the highest adsorption affinity to contamination among soil constituents [62]. Therefore, organic matter content is important for the adsorption and decay of organic molecules, and it is generally observed that it is most important in the topsoil and decreases significantly with depth. Natural processes in the soil such as decaying vegetation account for the higher organic matter content near the land surface. In addition to biomaterial, clay minerals are also one of the main components of soil and play an important role in the adsorption of contaminants [63]. Similarly, microbial activity is highest near the soil surface, especially around the root zone, and decreases with depth, resulting in a higher degradation rate at the upper soil depths and lower value at the deep soil depthsRamos et al., (2000). Therefore, depth-dependent reaction processes can strongly influence the fate and transport behavior of contaminants in the soil. Intrusion also of mostly saline mineral pollutants related to the contact between aquifers and the sea, constituting a boundary condition of subsurface environments with flows from the sea, can be enhanced by pumping exploitation of aquifers. The mixing zone between freshwater and intrusive seawater is an important feature of subsurface environments, e.g., the concentration of solutes and density of the fluid varies across the mixing zone due to constant or variable reaction, which carries pollutants into the outflowing freshwater contributing to convective circulation in the subsurface environment. The salinity of seawater is between 10 and 35g/l and that of freshwater [64, 65].

The relationship between adsorption and uptake depends on the type of contaminants and soil. For contaminants, such as pesticides and fertilizers, salinity, adsorption is often considered the major reaction process and uptake is generally ignored in most studies. Adsorption and solute degradation are related to the content of matter, clay minerals and microbial activity [61]. Both organic matter content and microbial activity in soils are strongly depth dependent as they generally decrease with depth. The depth distribution

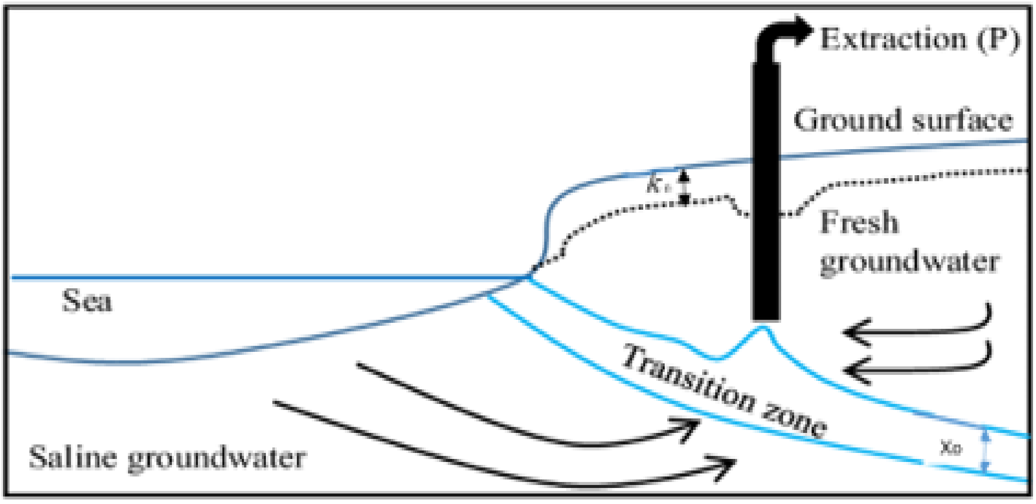

Figure 1.6: Evolution of salinity in groundwater. [65]

of organic matter and microbial activity is often found to be sigmoidal in shape. The following function adopted by [10] was used to represent spatially variable reactions:

$$k_d(x) = k_0 \cosh^{-2}(x/x_0) \tag{1.14}$$

Where $\cosh(x) = e^x + e^{-x}/2$ is the hyperbolic cosine function, is the adsorption coefficient in the topsoil, representing the maximum of$k_d(x)$,k_0 transition thickness between contaminated and fresh water. when the reaction is non-variable $k_d(x) = k_0$, here the linear depth-variable lag coefficient reduces to the term below:

$$R_d = 1 + \frac{\rho_b}{\theta} k_d(x) \tag{1.15}$$

Where θ is the porosity of the porous medium and the density of the medium.

1.5 Generalities on transport models of pollutants in underground media

1.5.1 Definition Models

A model is a simplified image of a complex reality that allows to simulate and extrapolate a reality . The general form of a model can be roughly represented as [66] follows:

$$\mu = F(\chi, L) + \eta \tag{1.16}$$

χ is the vector of input variables and μ is the vector of output variables. L is the vector of parameters to be taken into account and η is the error committed by assimilating the object of the study to its mathematically modeled image. lies in the assessment of the validity of the results according to the errors . A model must be accurate, robust, adaptable and simple to use as much as possible.

Types of Models

There are four major classes of models [66]:

- When F comes from experimentation, they are empirical models. Its name is rather used to define the way of obtaining certain laws, such as Darcy's Law, taken directly from the experiment, used in the calculation codes of the transfer models,
- Deterministic models correspond to a function F based on a certain mathematical and physical
- knowledge of the processes involved, in other words, the model is said to be deterministic when the physical properties of the system are introduced as they are supposed to exist in reality [67].
- When the input variables or parameters are considered as random functions, the models are said to be stochastic where the physical properties of the aquifer are described in the model by laws of spatial variability using statistical or geostatistical [68] tools.
- Black box models: this type of model is based on the determination of relationships between input and output data after analysis of the system, without the internal structure of the box being known.

1.5.2 Advection-dispersion equation models

Trace particles of pollutants are one of the main causes of hydro-environmental degradation in surface water bodies and aquifers. Solute particles reach a surface water body with sewage drainage and reach an aquifer due to seepage from waste disposal sites, underground septic tanks, mines, and polluted water bodies that recharge aquifers. Solutes are transported along the flow and disperse due to the combined effects of diffusion and advection [50]. Due to the increasing concern about the hydraulic environment for the existence of life on Earth, the advection-diffusion equation has attracted the attention of ecologists, hydrologists, civil engineers, and thematic modelers. Analytical and numerical solutions as well as the set of initial and boundary conditions of the advection-dispersion equation for real-life situations are useful in space and time, where the level of pollutant concentration will start to affect the health of inhabitants. In addition, such solutions allow estimating and examining the rehabilitation and management process of a polluted water body after removal approach without pollution interface [2]. The velocity of fluid flow is given by Darcy's law. When the soil is unsaturated, this velocity depends on the volumetric water content. The pollutant transfer equations take into account the water status of the soil and all the possibilities of changing the concentration [14]also taking into account the mobility of the chemical element, applying the principle of conservation of mass, the classical general equation of transport of a conservative chemical species with the one-dimensional flow in the subsurface medium is presented as follows [69]:

$$\underbrace{\frac{\partial(\rho s_i)}{\partial t}}_{a} + \underbrace{\frac{\partial(\theta c_i)}{\partial t}}_{b} = \underbrace{\frac{\partial}{\partial x}\left\{\theta D_i(\theta, q)\frac{\partial c_i}{\partial x}\right\}}_{c} - \underbrace{\frac{\partial}{\partial x}(qc_i)}_{d} + \underbrace{\sum_{j=1}^{n} \phi_{i,j}(c_i, s_i)_{c,i}(x,t)}_{e} \tag{1.17}$$

c_i is the concentration of the pollutant in the liquid phase, s_i is the concentration of the pollutant in the solid phase. D_i is the apparent diffusion coefficient of the chemical species, depending on the water content by volume and the Darcy flux given by equation (1.8). The first term (a) of the equation describes the rate of transition of the species (i) from the liquid to the solid phase and vice versa. from the liquid to the solid phase and vice versa; it includes the process of sorption/desorption and ion exchange. The second term (b) is the rate of accumulation of species (i) in the liquid phase. Term (c) describes the diffusive transfer combining molecular or ionic splitting with kinematic dispersion. Term (d) represents the convective transfer, the chemical species (i) being transported by the liquid flow. The term (e) takes into account the sources and consumptions of the species (i). Advection and dispersion represent two primary mechanisms that govern the transport of conservative solutes in a subsurface environment. Advection is the component of pollutant movement attributed to mean water flow in subsurface environments [13]. In other words, it is the transport of the dissolved solute at the average pore velocity of the fluid in the porous medium [53]. The phenomenon of dispersion can have several origins, including local heterogeneity of the real velocities of the fluid around the average value. Indeed, a particle will sample on its displacement a range of streamlines giving it an overall velocity different from its neighbor. Other factors such as the multiplicity of paths to get from point A to point B contribute to increase the dispersion of the tracer. In real case studies of contamination, the macroscopic to megascopic heterogeneity of the environment often makes it tedious to assess the velocity field, which is highly dependent on correct modeling of pollutant transport [14]. The use of the pollutant distribution coefficient allows the two S_i and C_i concentrations.k_d using the relationship between Si and Ci allows the introduction of the retardation function R into the transfer equation. The transport equation can then be rewritten as:

$$R\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_i\frac{\partial c}{x}\right) - \frac{\partial}{\partial x}(v_i c) + \varphi \tag{1.18}$$

Where $R = 1 + \frac{\rho_d}{\theta}k_d$ if the relationship between s and c is linear, then :$s = k_d c$,ρ_d is the dry density of the soil, θ porosity.

1.5.3 Fractional Advection-dispersion equation models

In recent decades, considerable attention to the fraction, calculus is increasingly increasing, although it has more than a four-hundred-year history Ghazal and Behrouz, (2020). This branch of calculus has allowed researchers to present the integration and differentiation of any arbitrary order . These advantages are used to model many real-world problems in terms of fractional-order differential equations [11]. Based on the fractional model in many fields, fractional derivatives can be used to describe many phenomena in different areas of engineering, physics, biology, medicine, economics, viscoelasticity, finance, chemistry, and fluid mechanics [70]. Many of these phenomena are modeled in terms of ordinary/partial differential equations of fractional order. This excellent tool is appropriate because many of the physical problems depend on the history of earlier times. Thus, obtaining the exact solution of fractional order partial differential equations (FPDEs) is more complex [11]. Fractional derivatives are also applicable to many physical problems especially involving dynamical systems where differential equations are involved [71]. Differential equations based on fractional derivatives are particularly well suited to describe anomalous dispersion processes, where a plume of particles propagates at a velocity incompatible with the classical Brownian motion model. When a fractional derivative replaces the second derivative in a diffusion or dispersion model, it leads to enhanced diffusion [72].

In this groundwater flow model, the second spatial derivative in the traditional ADE is replaced by a fractional derivative of order α, where $1 < \alpha < 2$.
Dispersion of aqueous tracers in natural systems, including heterogeneous soils, aquifers, and rivers, is generally in accord with a non-Fickian or anomalous mechanism. Non-Fickian transport behavior can be due to different mechanisms. In many studies, the diffusion process where diffusion takes place in a highly heterogeneous medium, numerous numerical experiments indicate that anomalous dispersion cannot be described by the traditional second-order ADE without extremely detailed information on the connectivity of high and low hydraulic conductivity sediments, proof that the ADE remains unsuitable in certain aquifers [11]. Environmental inhomogeneities can alter Markov diffusion laws in fundamental ways. In particular, the corresponding probability density of the concentration field may have a heavier tail than the Gaussian density, and its correlation function may decay from zero at a much slower rate than the usual exponential rate of Markov diffusion, resulting in long-range dependence. This phenomenon is known to be anomalous, and the fractional dispersion advection equation remains the only model adapted in all aquifers to describe and characterize the contaminant level [6]. The fractional advection-dispersion equation arises when the integer order derivative in the classical ADE is replaced by a fractional order derivative in time or space. [26], derived the general fractional advection-dispersion equation to describe particle transport in subsurface media using the following approach:

$$\frac{\partial^{\gamma} c(x,t)}{\partial t^{\gamma}} = v_{0x} \frac{\partial c(x,t)}{\partial x} + D \frac{\partial^{\alpha} c(x,t)}{\partial x^{\alpha}} \tag{1.19}$$

Where c is the pollutant concentration,$v_0 x$ is the average flow velocity in subsurface media, D is the dispersion coefficient ,γ is a fractional order for the time derivative and for the spatial derivative with $0 < \gamma < 1$ and $1 \prec \alpha \leq 2$. According to the approach conducted by [26], the fractional advection-dispersion equation is classified into this order: The spatial fractional ADE (γ=1 and $1 \prec \alpha \leq 2$), temporal fractional ADEs ($\alpha = 2$ and ($0 \prec \gamma \leq 1$), and spatio-temporal fractional ADEs ($0 \prec \gamma \leq 1$ and$1 \prec \alpha \leq 2$). The spatial fractional ADEs are appropriate for modeling particles with variable velocity, while the temporal fractional ADEs are appropriate for modeling particles with long rest time. The three forms of fractional advection-dispersion equations are presented below [26], Fractional advection-dispersion equation in space:

$$\frac{\partial c(x,t)}{\partial t} = v_{0x}\frac{\partial c(x,t)}{\partial x} + D\frac{\partial^{\alpha} c(x,t)}{\partial x^{\alpha}}, 1 \prec \alpha \leq 2 \tag{1.20}$$

Fractional advection-dispersion equation in the time

$$\frac{\partial^{\gamma} c(x,t)}{\partial t^{\gamma}} = v_{0x}\frac{\partial c(x,t)}{\partial x} + D\frac{\partial^{2} c(x,t)}{\partial x^{2}}, 0 \prec \gamma \leq 1 \tag{1.21}$$

Space-time fractional advection-dispersion equation

$$\frac{\partial^{\gamma} c(x,t)}{\partial t^{\gamma}} = v_{0x}\frac{\partial c(x,t)}{\partial x} + D\frac{\partial^{\alpha} c(x,t)}{\partial x^{\alpha}}, 0 \prec \gamma \leq 1, 1 \prec \alpha \leq 2 \tag{1.22}$$

In general, a lot of attention is paid to the space-time fractional differential equations, as it plays a very important role, especially in explaining the solute transport process in natural porous media with different degrees of heterogeneity [27].

1.5.4 Models of Boundary conditions

A numerical model can only work if we define boundary conditions, i.e. at the limits of the domain. From then on, the model is conditioned by the fact that the fluid enters or leaves at these boundaries Bahareh and Behrouz,(2021). It is necessary to specify and analyze the soil parameters as well as the data that express the initial state (t=0). The boundary conditions are of three forms:

- "Dirichlet" type condition: definition of quantities imposed on the artificial boundaries
- Neumann" or flow condition: definition of a flow linked to an effective precipitation, irrigation,

- drainage and impervious surface Cauchy" or mixed condition: definition of a transfer, function of a predefined elevation (water table/river interface, ...).

1.6 Generalities on numerical methods

The numerical resolution of the model can soften the conditions too idealistic for the analytical resolution, they allow to take into account more complex heterogeneous systems, they can be more realistic and flexible to simulate real conditions. The mathematical equations that deal with a partial derivative function are called PDEs [73]. It is not very obvious to obtain an analytical solution of linear PDE. However, there is an approximate solution of linear PDE obtained from different numerical methods [28]. Therefore, to solve the PDE of pollutant transport in porous media, different numerical methods are used. The finite difference method, Runge Kutta methods of order four Euler implicit method, based on an approximation of Grunwald and Caputo-Liousville, which are those used in this work.

1.6.1 Finite difference methods, finite volumes, finite elements and their advantages

Generally, finite difference methods are the most commonly used for the resolution of the flow problem. Detailed studies on the application of classical solution techniques to hydrogeological problems in subsurface environments have been developed by [74]. Each of these methods has its advantages and disadvantages. The difference and finite volume methods allow the calculation of the average load per mesh. They provide an exact mass balance at each element. The discretization of the flow equation by finite differences is obvious and simple to implement, but applicable only on rectangular or cubic meshes . Similarly, the finite volume method on a triangular mesh requires triangles conforming to the Delaunay principle. This principle is difficult to apply in the case of tetrahedra. Therefore, the finite difference and finite volume approaches are not appropriate for solving problems where the hydraulic conductivity is represented by a discontinuous solid tensor in space. The finite element method consists in reducing the hydraulic load by polynomials of degrees greater than or equal to one. Contrary to the finite difference and finite volume methods, the finite element method allows to discretize domains with complex geometry. This approach also comfortably handles cases where the hydraulic conductivity tensor is full. However, the flows are not determined unanimously between two adjacent elements [76]. With finite difference, finite volume, and finite element methods, the calculation of the flow velocity can generate additional errors especially when the load gradient is small to allow a direct and more accurate calculation of the flows.

1.6.2 Runge-Kutta method of fourth order and its advantages

The Runge-Kutta method of order 4 (RK4), remains nowadays a very powerful tool for the solution of ordinary differential equations (ODE) [77]. These are single-step methods, directly derived from Euler's method, which is an RK1 method. Most of the research has been directed towards improving the accuracy or the flexibility (to address problems of various nature) of the classical Runge-Kutta method. They have the advantage of being simple to program and quite stable for common physics functions. In terms of numerical analysis, they have the great advantage of not requiring anything other than the knowledge of initial values. It also has the advantage of compensating for the cumulative rounding error and reducing storage requirements compared to other numerical schemes [77, 79]. Runge-Kutta methods are also high-level methods, obtained from numerical integration formulas. Among the Runge-Kutta family of methods, the fourth-order method is the most widely used [73].

1.6.3 Euler implicit method, based on fractional derivatives

The Grunwald-Letnikov approach is based on the generalization of the fractional integer derivative. Let us consider the nth-order derivative of a function g defined on R as:

$$g^{n}(t)=\frac{d^{n}g}{dt^{n}}=\lim_{h\to 0}\frac{1}{h^{n}}\sum_{i=0}^{n}(-1)^{i}\begin{pmatrix} n \\ i \end{pmatrix}g(t-ih) \tag{1.23}$$

The generalization by allowing a n to be an arbitrary real or complex number will lead us to the Grunwald -Letnikov definition for fractional derivatives Zhang et al, (2016). Let g be a continuous defined on R; then the Grunwald-Letnikov fractional derivatives are defined as $\forall t, \alpha \in R$ follows :

$$ {}_{\alpha}D_{t}^{\alpha} g(t) = \lim_{h\to 0} h^{-\alpha} \sum_{i=0}^{\left[\frac{t-\alpha}{h}\right]} (-1) \begin{pmatrix} \alpha \\ i \end{pmatrix} g(t-ih), \alpha \prec t, \tag{1.24} $$

$$ {}_{t}D_{b}^{\alpha} g(t) = \lim_{h\to 0} h^{-\alpha} \sum_{i=0}^{\left[\frac{b-t}{h}\right]} (-1)^{i} \begin{pmatrix} \alpha \\ i \end{pmatrix} g(t-ih), b \succ t, \tag{1.25} $$

Where $\left[\frac{t-\alpha}{h}\right]$ denotes the integral part of$\frac{t-\alpha}{h}$, and

$$ D_{x}^{\alpha} c(x,t) = h^{-\alpha} \sum_{k=0}^{\left[\frac{x}{h}\right]} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} c(t-(k-1)h,t), \tag{1.26} $$

Standard Grunwald estimates generally give unstable finite difference equations, because the resulting finite difference method is either explicit or implicit [71]. Therefore, one can use a shifted Grunwald formula which is defined as follows: $\forall x \in R_{+}^{*}$

$$ D_{x}^{\alpha} c(x,t) = h^{-\alpha} \sum_{k=0}^{\left[\frac{x}{h}\right]} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} c(t-(k-1)h,t), \tag{1.27} $$

The Riemann-Liouville approach to the definition of the fractional derivative is based on the repeated integration of a continuous function g. The fractional Riemann-Liouville derivatives of a continuous function f defined on R, with are defined below:$\forall t \in R$ and $n \in N^{*}$

$$ {}_{\alpha}D_{t}^{\alpha} g(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^{n}}{dt^{n}} \int_{\alpha}^{t} (t-\tau)^{n-\alpha-1} g(\tau) d\tau, n-1 \leq \alpha \prec n, \alpha \prec t \tag{1.28} $$

$$ {}_{t}D_{b}^{\alpha} g(t) = \frac{1}{\Gamma(n-\alpha)} \left(-\frac{d}{dt}\right)^{n} \int_{t}^{b} (\tau-t)^{n-\alpha-1} g(\tau) d\tau, n-1 \leq \alpha \prec n, b \succ t \tag{1.29} $$

where$\Gamma(.)$ is the gamma function Caputo's approach to the definition of the fractional derivative is based on the repeated integration of a continuous function g, where$g \in c^{n}(R)$ and $\alpha \in R_{+}^{*}$ are defined as Lui et al,(2012): $\forall t \in R$ and $n \in N^{*}$

$$ {}_{\alpha}D_{t}^{\alpha} g(t) = \frac{1}{\Gamma(\alpha-n)} \int_{\alpha}^{t} (t-\tau)^{n-\alpha-1} g^{(n)}(\tau) d\tau, n-1 \leq \alpha \prec n, \alpha \prec t \tag{1.30} $$

$$ {}_{t}D_{b}^{\alpha}g(t) = \frac{(-1)^{n}}{\Gamma(\alpha - n)} \int_{t}^{b} (\tau - t)^{n-\alpha-1} g^{(n)}(\tau) d\tau, n-1 \leq \alpha \prec n, b \succ t \tag{1.31} $$

1.7 Conclusion

This chapter has allowed us to have a global view of the philosophy and progress of the functioning of underground environments and the mechanism of dispersion of pollutants in these environments. The underground environments generated by the different types of aquifers remain to this day a major interest in the water supply of the populations in many countries of the world. Indeed, groundwater is often potable at the source and is fairly well distributed geographically. The exploitation of these waters requires a good knowledge of potability sites. However, the pollution of these environments does not facilitate this understanding. Therefore, several approaches such as the knowledge and the functioning of the physical parameters that govern the underground environment, and the modeling and simulation of the transport of pollutants in the underground environment can contribute to a better understanding of them.

CHAPTER II

METHODOLOGY MATHEMATICAL MODELING AND NUMERICAL SOLUTION OF POLLUTANT TRANSPORT EQUATIONS IN SUBSURFACE MEDIA

2.1 Introduction

Knowledge of the physical description of the parameters that govern underground environments, as well as the techniques used to solve the transport models of pollutants in these environments, facilitates the interpretation and analysis of the results obtained. This chapter presents first the physical parameters influencing the dispersion of the pollutant in the underground media, then the presentation of the different models of transport equations of the solutes in the underground media associated with the different types of initial conditions and limits, and finally the presentation of the various methods of resolution employed to reach the objective of the work of this research. First, the numerical resolution of the advection dispersion equation (ADE) model by the finite difference method and Runge Kutta of order four and the numerical resolution of the Fractional dispersion advection equation (FADE) model by the Euler implicit method, based on an approximation of Grunwald-Letnikov and Riemann-Liouville, Caputo.

2.2 Physical description and modelling of the physical parameters governing underground environments

2.2.1 Dispersion coefficient

Dispersion is a physical phenomenon that occurs when moving away from the injection site, the mass of solute dilutes with time to occupy an increasing volume with a correspondingly decreasing concentration see Figure 2.1.

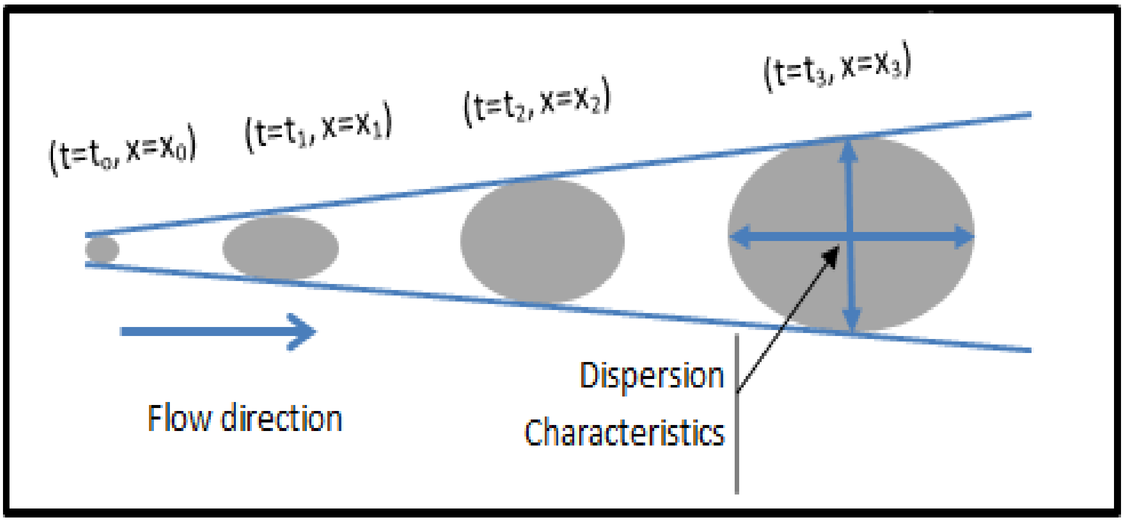

Figure 2.1: Geometry of the time-dependent dispersion problem.

a) Constant dispersion coefficient

The mechanisms of diffusion and kinematic dispersion give rise to the term: hydrodynamic dispersion (or simply dispersion). Assuming that dispersion transport represents mixing phenomena in accordance with Fick's law, [54]. In the case of an isotropic medium and a one-dimensional flow, the writing of the dispersion is simplified to:

$$D_e = \tau D_e + \alpha_L v_{0x} \tag{2.1}$$

Where τ is the Tortuosity of the subsurface medium , D_e is the effective dispersion coefficient and α_L is the longitudinal dispersivity of the subsurface medium.

b) Variable coefficient

Field and experimental evidence from studies have been suggested by [15–19] ofispersion is not constant but apparently increases as a function of displacement over time or equivalently with the distance of solute movement. The apparent increase in the coefficient of dispersion has been called the scaling effect by [80]. The scaling effect is generally attributed to the heterogeneity of the pore formation, particularly in the heterogeneity of the hydraulic conductivity. Stochastic analyses have shown that dispersivity depends on travel time and increases until it reaches an asymptotic value [20], and the theoretical deterministic analysis of [18] have also established that dispersivity in a stratified aquifer is time dependent. Therefore, there is ample evidence that the scale of dependence causes the variation of dispersion over time. Therefore, a time-dependent dispersion model can be used to provide an approximate description of the scale by operating the pollutant transport equation in subsurface media.

c) Time dependent coefficient of dispersion

- **Time-dependent linear dispersion function:** The time-dependent linear dispersion increases with time without boundary conditions in the porous medium [4, 58]. The linear formula for the time dependent dispersion expression in equation (8) is given by equation (2.2) below:

$$D(T)_L = D_0 \frac{T}{k_L} + D_m \tag{2.2}$$

- **Asymptotic dispersion function dependent on time:**

  The time-dependent asymptotic distance initially increases with time and eventually approaches an asymptotic value in the porous medium [58]ormula for time-dependent asymptotic dispersion expression is given by equation (2.3) below:

$$D(T)_A = D_0 \frac{T}{T + k_A} + D_m \tag{2.3}$$

  Where D_0 is the maximum dispersion coefficient for the asymptotic time-dependent and uniform dispersion function for the linear time-dependent dispersion coefficient; D_m is the effective diffusion coefficient of time; K_A is the time-dependent asymptotic coefficient equivalent to the mean distace travelled by the pollutants in the aquifer;K_L is the linear coefficient depending on time. The values of the parameters of the time-dependent dispersion coefficient were determined by a sensitivity analysis of [81].

d) Variable dispersion coefficient depending on the depth of the underground environment.

The variation of many subsurface parameters caused by natural disaster makes it difficult to use the advection dispersion equation with a single parameter to predict the concentration of contaminants at different distances in a porous medium. The asymptotic dispersivity is a physical quantity considered to account for the heterogeneity of porous media. Asymptotic dispersivity, which depends on the distance travelled by the fluids, is used to define the notion of a distance-dependent dispersion model for solute transport in heterogeneous porous media

[25, 52]. The hydrodynamic dispersion coefficient D (x) which is a function of the distance in the homogeneous porous medium in the absence of any molecular diffusion due to very fine tortuosity is written as equation (2.4) below:

$$D(x) = D_0 + \alpha(x)v_{0x} \tag{2.4}$$

Where $\alpha(x)$ is the dispersivity and $D_0 = [D_e\tau]$ is the molecular diffusion caused by molecular motion and particle collisions; with $\tau \leq 1$: tortuosity of the porous medium, is the effective dispersion. Asymptotic dispersivity is responsible for the heterogeneity of porous media and it initially increases with the distance traveled and eventually approaches an asymptotic value, [53]. Since the asymptotic dispersion coefficient depends on the distance, such a relation can be expressed equation (2.5) below:

$$D(x) = D_0 + \alpha\left(1 - \frac{b}{x+b}\right)v_{0x} \tag{2.5}$$

Where a is the value of the asymptotic dispersivity and b is a characteristic distance which determines the distance of displacement for the dispersivity to reach half of the asymptotic value. Dispersivity is the ratio of the asymptotic dispersion coefficient to the pore velocity of water. The values of b depend on the extent of the pre-asymptotic zone [18].

2.2.2 Physical description of the reaction coefficient

Studies of the flow and transport of contaminants in the underground environment rely on knowledge of many functional parameters of the subsoil. The delay factor generated by nonlinear absorption is one of these parameters inheriting significant ambiguities in its estimation in heterogeneous media. [13].

a) Physical description of the reaction coefficient

Studied in fractured media. However little information on non-linear sorption is available in the literature. Moreover, a transport model including nonlinear sorption at the scale of a single fracture has been developed by [13, 60] . Abulaban et cal. 1998 showed that below a threshold concentration value, the lag factor increases with the Freundlich isothermal exponent n, while the trend is reversed and the lag factor decreases when increases above this specific concentration. Due to the hydrodynamic dispersion, the concentrations in the plume decrease towards the edges of the plume. The delay factor model depending on the nonlinear absorption is given by the relation:

$$R_d = 1 + \frac{\rho_b}{\theta_m} k_d n c^{n-1} \tag{2.6}$$

k_d is the adsorption coefficient and n is the sorption intensity. (ρ_b) is the specific weight of the solid particle in the matrix, θ is the porosity of the porous medium (The porosity is the ratio between the volume of all the pores of a sample of the soil representative of the medium considered, and the total volume of the same sample). k_d expresses the ratio between the amount of solute concentration absorbed per unit area and the amount of concentration in solution. It eventually causes a delay of solute relative to mobile fluid in the fracture. The delay factor increases with the Freundlich isothermal exponent n. The retardation coefficient increases non-linearly with decreasing concentration. The effect of the isothermal exponent on the lag coefficient depends on the order of magnitude of the concentration. [60]

b) Variable reaction coefficient depending on the depth of the underground medium

As chemicals are transported through the soil, local reaction processes change with depth and differentiate in topsoil and subsoil. We have not yet found a physical consideration for the phenomenon of reaction variation with depth. However, the experimental studies carried out by [10] based on a series of experimental data on agricultural soils from various regions of the United States showed that the depth distribution of organic matter and microbial activity is sigmoidal in shape. Based on reality observed experimentally by [10], a depth-dependent reaction function has been adopted below to reflect the combined effects of organic matter and clay minerals on the change in adsorption coefficient with soil depth. The depth distribution of organic matter and microbial activity is sigmoidal in shape. The variable adsorption function is presented as follows:

$$k_d(x) = k_0 \cosh\left(\frac{x}{x_0}\right) \tag{2.7}$$

x_0 is a distance between contaminated water and fresh water which determines the rate at which reactions decrease with increasing depth. The depth dependent adsorption function describes the data well, since there is only one adjustable parameter, namely the depth x_0 transition. k0 is the adsorption coefficient in the topsoil, representing the maximum of k(x).

c) First-order decay coefficient

A first-order equation is used to represent the kinetics of simple reactions such as certain microbial degradation reactions. The equation (2.8) is written as:

$$\frac{\partial c}{\partial t} = -\lambda c \tag{2.8}$$

Where c is the concentration in the liquid phase, is the degradation coefficient which is expressed as a function of the half-life of the compound:

$$\lambda = \frac{\ln(2)}{T_{1/2}} \tag{2.9}$$

Where $T_(1/2)$ is the half-life time. The degradation kinetics of organic pollutants strongly depend on the properties of the medium (presence of an electron sensor, such as oxygen). Moreover, the kinetics observed for certain conditions is not necessarily transposable to other conditions, Gillham and O'Hannesin (1994).

2.3 Description and Mathematical Model.

Solute transport in groundwater systems is traditionally modeled by the classical advection-dispersion equation on the one hand, which can be added to an equilibrium absorption, the dispersion coefficient in all its forms and a first-order decay [82]. On the other hand, the fractional advection-dispersion equation (FADE), which plays a very important role, especially to explain the process of solute transport in natural porous media with different degrees of heterogeneity.

2.3.1 Advection-dispersion equation models

The advection-dispersion equation (ADE) is the most widely used method for modeling contaminant transport in subsurface environments. It describes the transport processes of contaminants in homogeneous porous media. The traditional advection-dispersion equation represents a standard model for predicting solute concentration in an aquifer based on mass conservation and Fick Bear's

on law, [80] and Combarnous, (1971). Four models of reactive solute transport are exploited depending on the nature of the medium through which the pollutants pass. These models are the (ADE), the (ADE) with distance-dependent dispersivity, the (ADE) with delay coefficient and distance-dependent dispersivity and the non-linear (ADE) with time-dependent dispersivity (Burgers equation). These models are detailed below.

Model 1: The advection-dispersion equation (ADE) with constant dispersivity: ADE for one-dimensional conservative pollutant transport with stable and saturated flow is presented below:

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v_{0x}\frac{\partial c}{\partial x} \tag{2.10}$$

where c is the concentration of the pollutant, is the average pore velocity taken in the direction of flow, x is the distance, and t is the time.$D = \tau D + \alpha_L v_{0x}$ is the hydrodynamic dispersion coefficient and represents a quasi-diffusion coefficient that accounts for both mechanical dispersion and molecular diffusion.

Model 2. The advection-dispersion equation (ADE) with distance-dependent dispersivity coefficient: Figure 2.2 illustrates the physical model of the problem. In this model, dispersion coefficient varies with respect to the depth, x, one-dimensional and the Darcy velocity is constant. The boundary conditions are defined at the boundaries of the matrix.

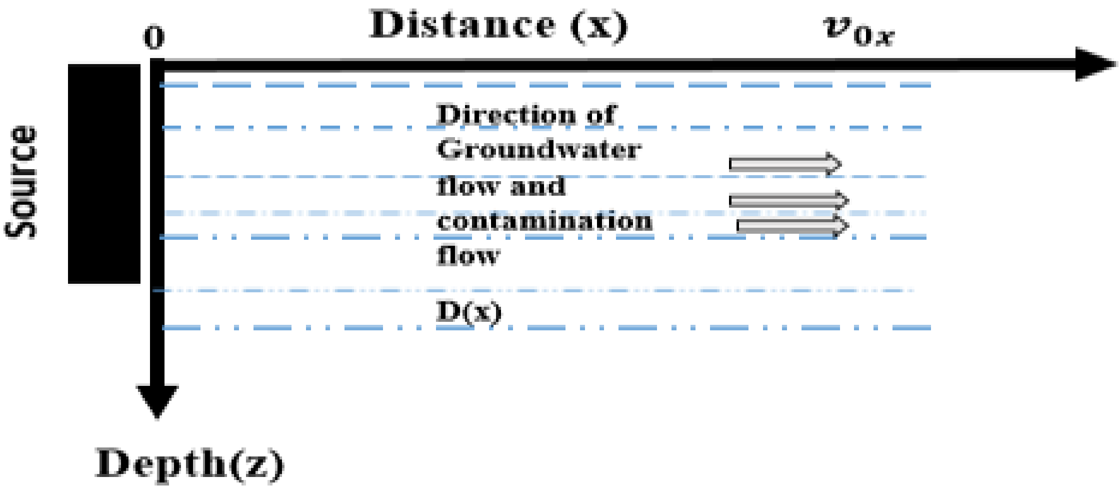

Figure 2.2: Physical model of the system.

The heterogeneity of most geological materials is caused by certain natural deformations, such as fractures, and lenses of high or low permeability which are at the origin of the variation of the hydraulic properties and the spatial or temporal increase of the dispersivity in the porous medium [52]. Field and experimental evidence from studies has been suggested by [18] that the dispersion coefficient is not constant but apparently increasing with time displacement and distant traveled by the solute. The phenomenon of dispersion is a phenomenon which moves away from the place of injection, the mass of solute is diluted during its displacement along the direction of flow x to occupy an increasing volume with a relatively decreasing concentration. The latter suggests that in a heterogeneous medium the pollutants transport equation taking into account a constant dispersion parameter become unsuitable, for this reason the distance-dependent dispersion coefficient is applied in the advection-dispersion equation below [25] .

The transport equation, defining the variation in concentration as a function of time and space of a dissolved substance transferred into a heterogeneous saturated porous medium, is written as the linear equation (2.11) form [8, 14] :

$$R\frac{\partial c}{\partial t} = D(x)\frac{\partial^2 c}{\partial x^2} - v_{0x}\frac{\partial c}{\partial x} \tag{2.11}$$

Where D(x) is the variable coefficient of dispersion as a function of the thickness x with $D(x) = D_0 + \alpha(x)v_{0x}$, with v_{0x_0x} fluid flow velocity. This equation involves two major terms influencing the transfer potential of the solute through a saturated porous medium. c is the concentration of the pollutants, R a retard factor generated by the absorption of the pollutant, t time and x distance traveled by the fluid in the porous medium. Convection or fluid flow velocity (v_0x) describes the transport of a solute by the movement of a fluid moving through a porous medium ; [4]. This water flow in a saturated porous medium (absence of gas in the pores) is defined by the following relation: $v_0x = q/ne$ or q = ki (Darcy flow) and ne: the effective porosity of the medium; k: the permeability of the aquifer, i: the hydraulic gradient of the aquifer (Figure 2.2).

Model 3. The advection-dispersion equation the (ADE) with distance-dependent reaction and dispersion coefficient:

Figure 2.3 illustrates the physical system of the problem: the unidirectional horizontal flow of fresh water through an aquifer of finite length L. In this physical system, the dispersion coefficient varies with depth x. This leads to fluctuations in the speed of the fluid, and eventually gives rise to adsorption which increases with distance.

The inhomogeneity of geological materials caused by irregular stratifications, cracks and faults cause spatially varying hydraulic properties, resulting in fluctuations in fluid velocity, and ultimately result in increasing dispersivity and reaction with increasing frequency of distance. The one-dimensional transport equation of pollutants in the aquifer with variable absorption and dispersion coefficients is given by the following linear relationship [1, 14, 28] :

$$R(x)\frac{\partial c}{\partial t} = D(x)\frac{\partial^2 c}{\partial x^2} - v_{0x}\frac{\partial c}{\partial x} \tag{2.12}$$

$R(x)$ is the retardation factor generated by the variable adsorption coefficient k(x) , c the concentration of contaminants.

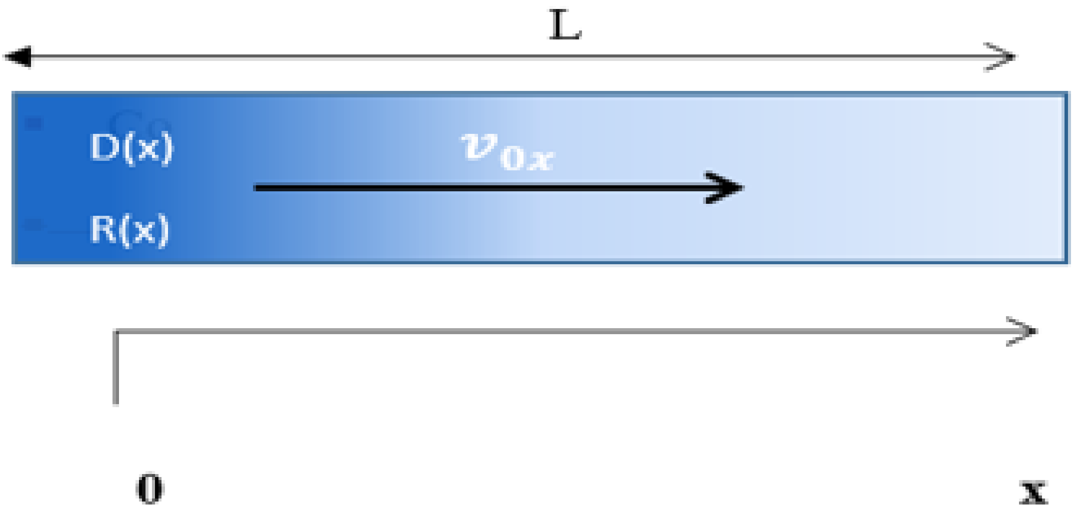

Figure 2.3: Physical system model.

Model 4. The nonlinear advection-dispersion equation (ADE) with time-dependent dispersivity coefficient (Burgers equation):

Water containing pollutants such as sewage eventually seeps into the aquifer which is a reservoir of drinking water. As water passes through the soil, pollutants are mixed, adsorbed, dispersed and diffused by the flowing stream Figure 2.4. Several efforts are being made by the scientific community to develop more precise and economical models capable of predicting the transport and concentration of solutes in unsaturated soils. The transport and mixing of contaminants is governed by the advection and dispersion equation of pollutants in the terrestrial aquifer [1].

Over the past decades, a large number of analytical and numerical solutions have been developed to estimate the fate and transport of various constituents in the underground environment. The application of these solutions is generally limited to non-variable subterranean flow fields and relatively simple initial and boundary conditions nevertheless; these solutions play an important role in contaminant transport studies, providing initial or rough estimates of the distribution of solute concentrations in soils and aquifer systems. The convection-dispersion equation has remained the basis of most analytical and numerical studies of solute transport. The dispersion equation which describes the distribution of the concentration of miscible fluids (i.e. water contaminated or salted with fresh water) in heterogeneous underground media remains one-dimensional in the direction of flow fluids along the x axis (ox) and the other oy and oz components become

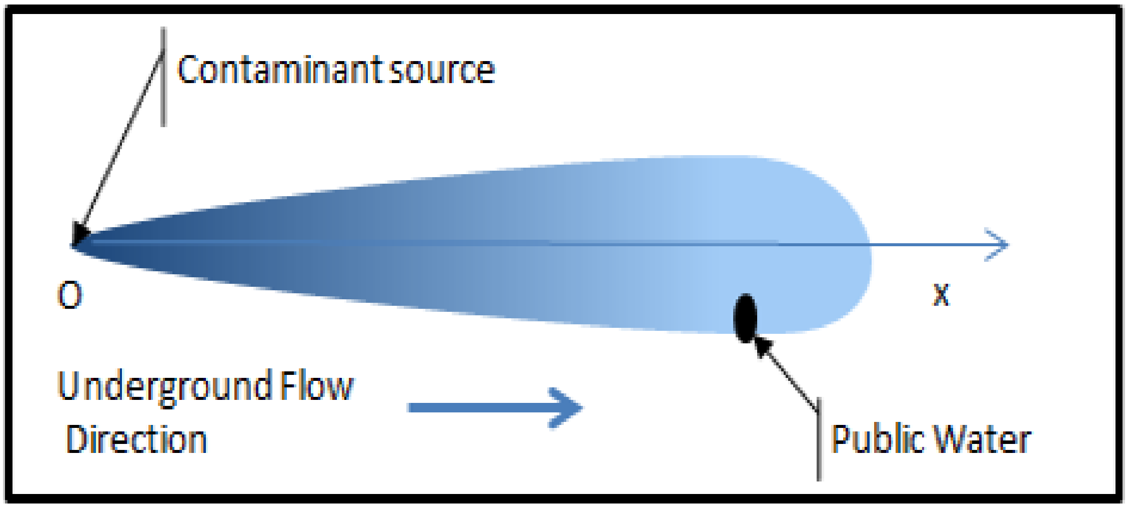

Figure 2.4: Infiltration and dispersal system of pollutants in the porous medium.

negligible. The transport equation can be written as equation (1.13) [3, 83], :

$$\frac{\partial c}{\partial t} + \left(\frac{1-\phi}{\phi}\right)\frac{\partial F}{\partial t} = D_L\frac{\partial^2 c}{\partial x^2} - v_{0x}\frac{\partial c}{\partial x} \tag{2.13}$$

Where c is the concentration of the contaminated fluid, F is the concentration in the solid phase, ϕ the porosity of the medium, with DL the longitudinal dispersion coefficient on the macroscopic scale, and (v_0x) the component of the infiltration rate of salt water along the x-axis, and DL is the length of dispersion in the direction of flow. Two cases were considered by [84] for the solid phase concentration and its derivative, which are equations (2.14) and (2.15):

$$F = k_1c + k_2 \tag{2.14}$$

$$\frac{\partial F}{\partial t} = k_1c - k_2F \tag{2.15}$$

Here there is an equilibrium and unbalanced relationship between the concentrations in the two phases. k_1 and k_2 are the constants generally referred to as the order factor for the distribution of pollutants in aquifers. By combining the equations (2.14) and (2.15) in (2.13), we obtain equation (2.16):

$$R\frac{\partial c}{\partial T} = D_L\frac{\partial^2 c}{\partial X^2} - v_{0x}\frac{\partial c}{\partial X} \tag{2.16}$$

Where R is the delay factor describing the absorption of solutes in the porous medium, its expression is equation (2.17):

$$R = \left(1 + \frac{1-\phi}{\phi} k_1\right) \tag{2.17}$$

The component of the infiltration rate is related to the dispersal concentration of the pollutant. [2]assumes that the rate of infiltration is inversely proportional to the concentration of the pollutant as given in equation (2.18):

$$v_{0x} = \frac{c(x,t)}{c_0} \tag{2.18}$$

This infiltration rate is the cause of the nonlinearity in the advection ? dispersion equation. $\frac{1}{c_0}$ represents the proportionality concentration of salt water dispersion. The new parameters of the independent variables introduced to simplify equation (2.16) are defined as $T = \frac{Rt}{L}$ and $X = \frac{xc_0}{L}$ .Therefore, equation (2.16) reduces to equation (2.19):

$$\frac{\partial c}{\partial T} = D_L \frac{\partial^2 c}{\partial X^2} - c\frac{\partial c}{\partial X} \tag{2.19}$$

Introduction of the time-dependent dispersion model in the burger equation

Field and experimental evidence from studies have been suggested by [18, 19]; that the dispersion coefficient is not constant but increasing as a function of the displacements in time or equivalently with the distance of displacement of the solute. The apparent increase in the dispersion coefficient has been called the scale effect [80]. The scale effect is generally attributed to the heterogeneity of the porous formation, in particular in the heterogeneity of the hydraulic conductivity. Stochastic analyzes have shown that the dispersion depends on the transport time and increases until it reaches an asymptotic value [20]. The theoretical deterministic analysis of [85] also established that the dispersivity in a stratified aquifer is time-dependent. Therefore, there is ample evidence that the dependency scale causes dispersion to vary over time. Therefore, a time-dependent dispersion model can be used to provide a rough description of the transport scale in our study by exploiting the Burger equation. In this study, a linear and asymptotic form of the time-dependent dispersion coefficient is integrated into the nonlinear PDE equation

(7) to study the phenomena of longitudinal dispersion of solutes in the underground environment; this has been mentioned in various works ([58, 86]. This type of dispersion will make it possible to better represent the results for the transport of solutes in a given porous medium. The time-dependent dispersion coefficient is studied in two forms in this work and equation (2.19) becomes equation (2.20):

$$\frac{\partial C}{\partial T} = D(T)_{L,A}\frac{\partial^2 C}{\partial X^2} - C\frac{\partial C}{\partial X} \tag{2.20}$$

where $D(T)_{L,A}$ is the time dependent dispersion presented first on the linear form

$$D(T)_L = D_0\frac{T}{k_L} + D_m \tag{2.21}$$

Asymptotic sequence

$$D(T)_A = D_0\frac{T}{T + k_A} + D_m \tag{2.22}$$

K_A is the time-dependent asymptotic coefficient equivalent to the mean distace travelled by the pollutants in the aquifer; K_L is the linear coefficient depending on time.

2.3.2 Advection-dispersion -fraction equation model

Pollutants infiltrating groundwater can be studied by integrating zero-order and first-order adsorption and decay coefficients. The movement of solute in the flow region occurs due to advection and dispersion. One-dimensional solute motion in a heterogeneous porous medium can be studied numerically using the spatial fractional advection-dispersion equation for a one-dimensional unsteady-state velocity field with a first-order decay function, and an absorption coefficient non-linear. s-FADE is a spatially nonlocal model capable of describing solute particle motions encompassing a very large transition due to high heterogeneity to preferential high-velocity flow paths. The influence of heterogeneity leads to the variability of some coefficients of the FADE model hence the fractional-order in this work is allowed to be variable in the porous medium, a fraction instead of the integer constant of 2. The one-dimensional advection-dispersion space-fractional equation for a conservative contaminant can be written as follows [13, 27]:

$$R_d \frac{\partial c(x,t)}{\partial t} = D_f \frac{\partial^\alpha c(x,t)}{\partial x^\alpha} - v_{0x} \frac{\partial c(x,t)}{\partial x} + \lambda c(x,t) \tag{2.23}$$

Where c is the concentration of the contaminant, D_f is the fractional dispersion coefficient, t is the time, and x is the distances traveled by the fluid in the porous medium. is the first-order decay coefficient and R_d is the retard factor generated by the nonlinear sorption of the pollutant. The temporal fractional advection-diffusion model can be written in the form of the following equation (2.24) [13]; :

$$\frac{\partial^\gamma c(x,t)}{\partial t^\gamma} = \frac{1}{R_d}\left[D_f \frac{\partial c(x,t)}{\partial x} - v_{0x} \frac{\partial c(x,t)}{\partial x} + \lambda c(x,t)\right] \tag{2.24}$$

2.4 Initial and boundary conditions for each model

- **Initial and boundary conditions for the 1 , 2 and fractional model**

Figure 2.5: Geometry of the problem.

From the source of the pollutants, the concentration disperses further into the porous medium in the direction of flow (x) figure 2.5. A one-way horizontal flow of water through an aquifer of finite length L is considered [28]. The problem can be mathematically defined by equations 1 and 2 with the initial and boundary conditions given successively in equations (2.25) and (2.26) as follows:

$$C(x,0) = 0, 0 \prec x \leq L, \tag{2.25}$$

$$\begin{cases} C(0,t) = C_0, \forall t \geq 0 \\ \frac{\partial C(L,t)}{\partial x} = 0, \forall t \succ 0 \end{cases}, \tag{2.26}$$

- **Initial and boundary condition for model 3**

The initial condition constants (a), variables exponentially with time (b) and sinusoidally with time (c) were introduced at the inlet of the aquifer (initial injection concentration). The problem can be defined mathematically by model 3. with the following initial conditions and boundary conditions [4]

$$\begin{cases} c(L,0) = 0; for, 0 \prec x \leq L \\ c(0,t) = c_0; , if, t \geq 0 \\ \frac{\partial c(L,t)}{\partial x} = 0, if, t \geq 0 \end{cases} \tag{2.27}$$

Where λ is the first order decay coefficient. The decay coefficient can be related to the half-life t1/2 of a decomposing material.

$$\begin{cases} c(L,0) = 0; for, 0 \prec x \leq L \\ c(0,t) = c_0 e^{-\lambda t}, if, t \geq 0 \\ \frac{\partial c(L,t)}{\partial x} = 0, if, t \geq 0 \end{cases} \tag{2.28}$$

The original periodic entry condition is assumed. This condition was chosen experimentally by Ebach and White (1958) where the considered the concentration at the entrance of the porous medium as the response of a harmonic function of time. The technical frequency response required the response to a sinusoidally varying input concentration. This is one of the unusual initial conditions adopted by [13]. The sinusoidal input shape was used to assess the behavior of pollutants in porous media as reported in previous research [4, 8]. The initial and limiting conditions considered are given as follows:

$$\begin{cases} c(L,0) = 0; for, 0 \prec x \leq L \\ c(0,t) = c_0 \left[1 + \sin(wt)\right], if, t \geq 0 \\ \frac{\partial c(L,t)}{\partial x} = 0, if, t \geq 0 \end{cases} \tag{2.29}$$

Where w is the pulsation differentiates the periodic wave fronts. This parameter was also exploited in the work of [4] to study the effects of time-dependent entry boundary condition.

- **Initial and boundary condition for model 4**

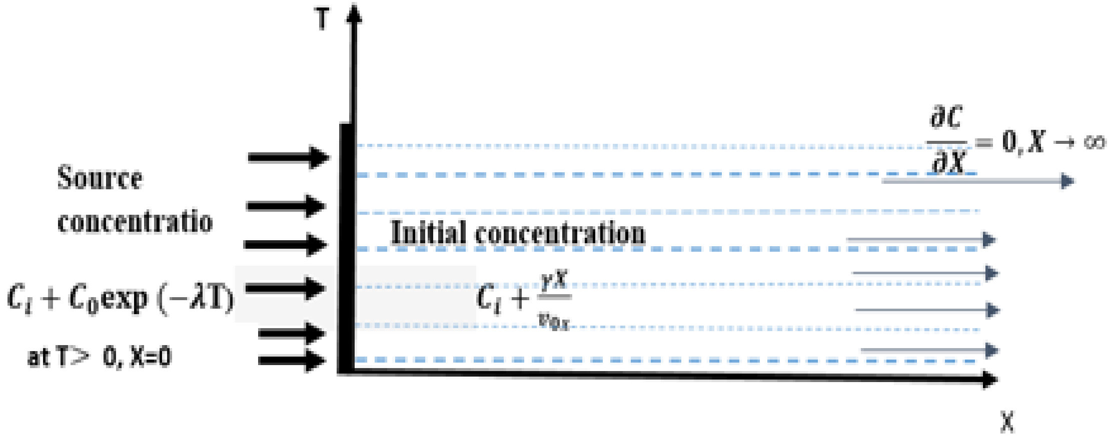

Figure 2.6: Geometry of the problem.

From the source of the pollutants, the concentration disperses more in the porous medium in the direction of flow with a front at the arrival of the boundary see Figure 2.6. At the initial moment it is assumed that the aquifer is contaminated, a certain initial background concentration exists in the aquifer and it is represented by a linear combination of an initial concentration and the term of zero order production with rapid infiltration given by equation (2.30):

$$c(X,0) = c_i + \frac{\gamma X}{v_{0x}}, X \succ 0, t = 0 \tag{2.30}$$

Where c_i is the initial background concentration, is flow velocity, and ? is the zero order production rate coefficient for liquid phase solute production.

A contaminant in radioactive waste decaying exponentially with time is imposed upon entering the aquifer as a linear combination of a source concentration with an initial background concentration at the origin, to describe the transport of solutes in a natural or artificial system as expressed by equation (2.31) [21, 82] :

$$C(0,T) = C_i + C_0 \exp(-\lambda T), T \succ 0; X = 0 \tag{2.31}$$

λ is the decay rate constant .

At the other end of the aquifer, solute transport may not be affected and therefore an exit boundary condition is prescribed as a non-flow boundary condition [21]. The mathematical expression of these phenomena is expressed by equation (2.32) as:

$$\frac{\partial C}{\partial x} = 0, x \rightarrow \infty \tag{2.32}$$

2.5 Numerical method

The one-dimensional solute transport equation is a parabolic-type partial differential equation in which, the finite difference technique is commonly used to obtain the numerical solution. An explicit finite difference technique is usually used, and eventually gives birth to restrictive stability criteria [21].

2.5.1 Numerical solution of the 1,2,3 model by the finite difference method

The derivatives of the 1,2,3 model of the dispersion advection equation are approximated by the truncated expansion of the approximation to the finite difference numerical scheme to determine the first and second order spatial derivatives are given according to this relations [13]:

$$\frac{\partial c}{\partial x} = \frac{c_i^j - c_{i-1}^j}{\Delta x} \tag{2.33}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{i+1}^j - c_i^j + c_{i-1}^j}{\Delta x^2} \tag{2.34}$$

The first order time discretization is given by the following relation:

$$\frac{\partial c}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t} \tag{2.35}$$

Subscripts (i) and (j) indicate discretization nodes along (x) and (t) respectively. Δx and Δt are the spatial and temporal steps, respectively. Thus, model (1) can be written in the following discrete form:

$$c_i^{j+1} - c_i^j = \frac{D\Delta t}{R\Delta x^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) - \frac{v_{0i}\Delta t}{R\Delta x}\left(c_i^j - c_{i-1}^j\right) \tag{2.36}$$

The numerical solution of model (2) is given in the following form:

$$c_i^{j+1} - c_i^j = \frac{D_i\Delta t}{R\Delta x^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) - \frac{v_{0i}\Delta t}{R\Delta x}\left(c_i^j - c_{i-1}^j\right) \tag{2.37}$$

$$c_i^{j+1} = (1 - 2\alpha - \beta)c_i^j + \alpha c_{i+1}^j - (\alpha + \beta)\, c_{i-1}^j \tag{2.38}$$

With $\alpha = \frac{D_i\Delta t}{R\Delta x^2}$ and $\beta = \frac{v_{0i}\Delta t}{R\Delta x}$;$D_i = D_0 + \alpha\left(1 - \frac{b}{x_i+b}\right)v_{0i}$

The numerical solution of model (3) is given in the following form:

$$c_i^{j+1} - c_i^j = \frac{D_i\Delta t}{R_i\Delta x^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^i\right) - \frac{v_{0i}\Delta t}{R_i\Delta x}\left(c_i^j - c_{i-1}^i\right) \tag{2.39}$$

$$c_i^{j+1} = \left(1 - 2\alpha_1 - \beta_1\right)c_i^j + \alpha_1 c_{i+1}^j + \left(\alpha_1 + \beta_1\right)c_{i-1}^i \tag{2.40}$$

With $\alpha_1 = \frac{D_i\Delta t}{R_i\Delta x^2}$ and $\beta_1 = \frac{v_{0i}\Delta t}{R_i\Delta x}$,$R_i = 1 + \frac{\rho}{\theta}k_0\cosh\left(\frac{x_i}{x_0}\right)$,$x = i\Delta x, t = j\Delta t$,where (i=0,1,2,...,Nx) and (j=0,1,2, ...,Nt) .

2.5.2 Numerical solution of the burger equation by the Runge Kutta method of order four

The numerical technique is used to solve the equation (2.20) expressed as equation (2.41) [73, 77, 87] :

$$\frac{\partial c}{\partial T} = f(T, c(T)), \tag{2.41}$$

The semidiscrete equation (2.41) is solved using the RK4 scheme according to the algorithm given by equation (2.42):

$$\begin{cases} K_1 = \Delta T f(T, c(T)) \\ K_2 = \Delta T f(T + \frac{1}{2}\Delta T, c(T) + \frac{1}{2}K_1) \\ K_3 = \Delta T f(T + \frac{1}{2}\Delta T, c(T) + \frac{1}{2}K_2) \\ K_4 = \Delta T f(T + \Delta T, c(T) + K_3) \\ c(T, \Delta T) = c(T) + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \end{cases} \tag{2.42}$$

With (ΔT) the time step, c (T) the value of the pollutant concentration at time t and c (T+ ΔT) the value of the pollutant concentration at time (T + ΔT). The derivatives of the model 4 are approximated by the truncated expansion of the numerical finite difference approximation scheme to determine the first and second order spatial derivatives are obtained from equations (2.43) and (2.44) ([13]):

$$\frac{\partial c}{\partial X} = \frac{c_i^j - c_{i-1}^j}{\Delta X}, \tag{2.43}$$

$$\frac{\partial^2 c}{\partial X^2} = \frac{c_i^{j+1} - 2c_i^j + c_{i-1}^j}{\Delta X^2}, \tag{2.44}$$

The first order temporal discretization is given by equation (2.45) written as:

$$\frac{\partial c}{\partial T} = \frac{c_i^{j+1} - c_i^j}{\Delta T}, \tag{2.45}$$

The indices (i) and (j) indicate the nodes of discretization along (X) and (T) respectively. Δx is the spatial step. Thus, equation (2.20) can be written in a discrete form such as equation (4.46):

$$\frac{\partial c_i^j}{\partial T} = f(X, T, c_{i+1}^j, c_i^j, c_{i-1}^j), \tag{2.46}$$

Where the function $f(X, T, C_(i+1)^j, C_i^j, C_(i-1)^j)$ in equation (4.46) is expressed as equation (2.47):

$$f(X, T, c_{i+1}^j, c_i^j, c_{i-1}^j) = D(j)\left(\frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{\Delta X^2}\right) - c_i^j\left(\frac{c_i^j - c_{i-1}^j}{\Delta X}\right), \tag{2.47}$$

$X = i\Delta X$,$T = j\Delta T$, With (i=0,1,2,...,Nx) and (j=0,1,2, ...,Nt) , $D(j)_L = D_0\frac{T_j}{K_L} + D_m$,$D(j)_A = D_0\frac{T_j}{T_j + k_A} + D_m$

2.5.3 Numerical solution of the fractional order advection-dispersion equation

a) Spatial fractional order derivative by the implicit Euler method, based on a Grunwald approximation

In this part, the basic theory of the numerical solution of the fractional space of equation (2.23) in an infinite domain is exploited [27]. The discrete approximation of the fractional derivative term can be defined from the Grunwald norm, as follows.

$$\frac{\partial^{\alpha} c}{\partial x^{\alpha}} = \frac{1}{\Gamma_{(-\alpha)}} \lim_{n \to \infty} \frac{1}{h^{\alpha}} \sum_{k=0}^{i} \frac{\Gamma_{(k-\alpha)}}{\Gamma_{(k+1)}} c(x - kh, t), \tag{2.48}$$

Where i is a positive index, $\Gamma_{(-\alpha)}$ is the gamma function. The value of the fractional derivative at a point x depends on the values of the function at that point and all points to the left of that point of interest x. The explicit Euler method associated with the Grunwald approximation on fractional derivatives will be used in this part, which is as follows:

$$\frac{c_i^{j+1} - c_i^j}{\Delta t} = \gamma c_i^j - v_{0x} \frac{c_i^j - c_{i-1}^j}{h} + \frac{D_f}{h^{\alpha} \Gamma_{(-\alpha)}} \sum_{k=0}^{i} \frac{\Gamma_{(k-\alpha)}}{\Gamma_{(k+1)}} c_{i-k}^j \tag{2.49}$$

were (i= 1,2,...,Nx), (k=0, 1,2, ...,) et (j=0, 1,2, ...,Nt) . Normalized Grunwald weights are defined by:

$$f_k = \frac{\Gamma_{(k-\alpha)}}{\Gamma_{(-\alpha)} \Gamma_{(k+1)}} \tag{2.50}$$

These normalized weights only depend on the order α and the index k. (For example, the first four terms of this sequence are given by :$f_0 = 1$, $f_1 = -(\alpha$, $f_2 = \alpha(\alpha - 1)/2\alpha$, $f_3 = \alpha(\alpha - 1)(\alpha - 2)/3!$, the resulting equation to be solved explicitly is reduced by:

$$c_i^{j+1} = \left(1 + \lambda - \frac{\Delta t}{h} v_{0x} + \frac{\Delta t}{h^{\alpha}} D_f\right) c_i^j + \left(\frac{v_{0x}}{h} + \frac{\alpha}{h^{\alpha}} D_f\right) \Delta t c_{i-1}^j + \frac{D_f}{h^{\alpha}} \sum_{k=2}^{i} f_k c_{i-k}^j \tag{2.51}$$

b) Derivative of temporal fractional order by the implicit Euler method, based on a Caputo-Liousville approximation

In this section, the solution of the temporal fractional numerical equation (2.24) in an infinite domain is developed. The Caputo-Liousville fractional derivative is exploited with the following equation [26]:

$$\frac{\partial^\gamma c}{\partial t^\gamma} = \frac{1}{\Delta t^\gamma \Gamma_{(2-\gamma)}} \sum_{k=0}^{j} w_k^\gamma \left[c(x, t_{j+1-k}) - c(x, t_{j-k})\right], \tag{2.52}$$

where $w_k^\gamma = (k+1)^{1-\gamma} - k^{1-\gamma}, k = 1, 2, ..., n$,(i=0, 1,2,..., Nx) et (j= 1,2, ..., Nt) . The explicit Euler method associated with the Caputo-Liousville approximation on the equation (2.24) is used in this part, which is presented by the following equation (2.53):

$$\frac{(R_d)_i^j}{\Delta t^\gamma \Gamma_{(2-\gamma)}} \sum_{k=0}^{j} w_k^\gamma \left[c(x, t_{j+1-k}) - c(x, t_{j-k})\right] = -\frac{v_{0x}}{h}\left(c_i^{j+1} - c_{i-1}^j\right) + \frac{D_f}{h^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) + \lambda c_i^j \tag{2.53}$$

By simplifying equation (2.53) we obtain the following equation (2.54) to be solved explicitly:

$$c_i^{j+1} = c_i^j - a_1 \sum_{k=1}^{j} w_k^\gamma \left[C(x, t_{j+1-k}) - c(x, t_{j-k})\right] - a_2\left(c_i^j - c_{i-1}^j\right) + a_3\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) \tag{2.54}$$

where $a_1 = w_0^{-\gamma}$,$a_2 = \frac{w_0^{-\gamma} v_{0x}}{b\Delta t}$,$b = \frac{(R_d)_i^j \Delta t^{-\gamma}}{\Gamma_{(2-\gamma)}}$, $a_3 = \frac{D_i w_0^\gamma h^{-2}}{b}$, $(R_d)_i^j = 1 + \frac{\rho_b}{\theta_m} k_d n (c^{n-1})_i^j$

$$c_i^{j+1} = \left(1 + \lambda - \frac{\Delta t}{h} v_{0x} + \frac{\Delta t}{h^\alpha} D_f\right) c_i^j + \left(\frac{v_{0x}}{h} + \frac{\alpha}{h^\alpha} D_f\right) \Delta t c_{i-1}^j + \frac{D_f}{h^\alpha} \sum_{k=2}^{i} f_k c_{i-k}^j \tag{2.55}$$

2.5.4 Discretization of the Initial and Boundary Conditions for the 1, 2 and fractional model

- **Discretization of the Initial and Boundary Conditions for the 1, 2 and fractional model** The discretization of the initial conditions and limit associated with the equation (2.25) and (2.26) to apply to this method is given successively to the following equation (2.56):

$$\begin{cases} c_i^0 = 0, 0 \prec i \leq k-1 \\ c_0^j = c_0, \forall j \geq 0 \\ \frac{\partial c_{N_x}^j}{\partial x} = 0, \forall j \geq 0 \end{cases} \tag{2.56}$$

- **Discretization of the Initial and Boundary Conditions for Model 3**

The discretization of boundary and initial conditions is necessary to apply this method. The discrete version of the initial and boundary conditions associated with the equation is expressed as:

$$\begin{cases} c_i^0 = 0, if, 0 \prec i \leq N_x \\ c_0^j = c_0\left[1+\sin(wt_j)\right], if, j \geq 0 \quad , \\ \frac{\partial c_{N_x}^j}{\partial x} = 0, if, j \geq 0 \end{cases} \tag{2.57}$$

$$\begin{cases} c_i^0 = 0, if, 0 \prec i \leq N_x \\ c_0^j = c_0 e^{-\lambda t_j}, if, j \geq 0 \quad , \\ \frac{\partial c_{N_x}^j}{\partial x} = 0, if, j \geq 0 \end{cases} \tag{2.58}$$

$$\begin{cases} c_i^0 = 0, if, 0 \prec i \leq N_x \\ c_0^j = c_0\left[1+\sin(wt_j)\right], if, j \geq 0 \\ \frac{\partial c_{N_x}^j}{\partial x} = 0, if, j \geq 0 \end{cases} \tag{2.59}$$

- **Discretization of the Initial and Boundary Conditions for Model 4**

The discrete version of the initial condition and boundary conditions associated with equation (2.30), (2.31) and (2.32) is expressed as equation (2.60):

$$\begin{cases} c_i^0 = c_i + \frac{\gamma X_i}{v_{0x}}, i \succ 0, j = 0, \\ c_i^0 = c_i + c_0\exp(-\lambda T_j), j \succ 0, i = 0 \\ \frac{\partial c_{N_x}^j}{\partial x} = 0, j \succ 0, \end{cases} \tag{2.60}$$

2.5.5 Stability conditions

a) Stability condition for model 2,3,4

- **Condition of stability for the model 2**

For an approach similar to that used by [13] where the spatial and temporal steps tend to zero, which also leads the error to tend to zero. This leads to imposing certain conditions on the finite difference scheme of the discrete equation (2.38) which are given by the following equation (2.61):

$$\begin{cases} 0 \leq 1 - 2\alpha - \beta \leq 1 \\ 0 \leq \alpha \leq 1 \\ 0 \leq \alpha + \beta \leq 1 \end{cases} \tag{2.61}$$

The new solution is a convex combination of the solution at new time step (j+ 1) at a spatial node i is an average of the solutions at the previous time step at the nodes i-1, i and i +1. The new solution linked continuously to the initial value ofc_i^0 is given by equation(2.62)

$$\begin{cases} \beta \leq 1 - 2\alpha \leq 1 + \beta \\ 0 \leq \alpha \leq 1 \\ -\alpha \leq +\beta \leq 1 - \alpha \end{cases} \tag{2.62}$$

By simplifying equation 2.62a and 2.62c we have $\beta \leq 1 - 2\alpha$ Thus, the stability conditions are $0 \leq \alpha \leq 1$and$-\alpha \leq +\beta \leq 1 - 2\alpha$ In this work $0 \leq \frac{D_i \Delta t}{R \Delta x^2} \leq 1$ and $-\frac{D_i \Delta t}{R \Delta x^2} \leq \frac{v_{0i} \Delta t}{R \Delta x} \leq 1 - \frac{D_i \Delta t}{R \Delta x^2}$

- **Stability condition for model 3**

$$\begin{cases} 0 \leq 1 - 2\alpha_1 - \beta_1 \leq 1 \\ 0 \leq \alpha_1 \leq 1 \\ 0 \leq \alpha_1 + \beta_1 \leq 1 \end{cases} \tag{2.63}$$

Then the new solution is a convex combination of the previous equation (2.63):

$$\begin{cases} \beta_1 \leq 1 - 2\alpha_1 \leq 1 + \beta_1 \\ 0 \leq \alpha_1 \leq 1 \\ -\alpha_1 \leq \beta_1 \leq 1 - \alpha_1 \end{cases} \tag{2.64}$$

Therefore $-\alpha_1 \leq \beta_1 \leq 1 - 2\alpha_1$

Thus, the conditions of stability are $-\alpha_1 \leq \beta_1 \leq 1 - 2\alpha_1$,$0 \leq \alpha_1 \leq 1$ and $-\alpha_1 \leq \beta_1 \leq 1 - 2\alpha_1$

In this work $0 \leq \frac{D_i \Delta t}{R_i \Delta x^2} \leq 1$ and $-\frac{D_i \Delta t}{R_i \Delta x^2} \leq \frac{v_{0i} \Delta t}{R_i \Delta x} \leq 1 - \frac{D_i \Delta t}{R_i \Delta x^2}$

- **Stability condition for model 4**

Equation (2.47) can be written in the discrete form as equation (2.65) below:

$$C_i^{j+1} = (1 - 2\alpha_2)C_i^j + \alpha_2 C_{i+1}^j + \alpha_2 C_{i-1}^j + \beta_2 C_i^j (C_i^j - C_{i-1}^j), \tag{2.65}$$

The coefficients α_2 and β_2 defined in equation (2.65) are presented successively in equation (2.66) and (2.67)

$$\alpha_2 = \frac{D_j \Delta T}{\Delta X^2}, \tag{2.66}$$

$$\beta_2 = \frac{\Delta T}{\Delta X}, \tag{2.67}$$

The coefficients determined in equation (2.65) make it possible to impose the following stability condition given by equation (25) below:

$$0 \leq 1 - 2\alpha_2 \leq 1, 0 \leq \alpha_2 \leq 1, 0 \leq \beta_2 \leq 1 \tag{2.68}$$

For the conditions of stability equation (2.68), the coefficients of the terms on the right must be positive, thus $\alpha_2 = \frac{D_j \Delta T}{\Delta X^2} \succ 0$and $\beta_2 = \frac{\Delta T}{\Delta X} \succ 0$ From equation 2.68 we obtain the stability condition which is expressed as equation (2.69) below:

$$0 \leq \Delta T \leq \frac{\Delta X^2}{2D_j}, \tag{2.69}$$

These inequalities fix a strict maximum limit to the size of the time step and represent a serious limitation for the centered finite difference diagram.

b) Stability condition for the advection-dispersion-fractional equation model

- **Stability condition for the spatial fractional order derivative**

Suppose that c_i^0 is the only term that has an error, so the perturbed value is $\underline{c_i^0} = c_i^0 + \delta_i^0$, this perturbation produces a perturbed value for given$\underline{c_i^1} = c_i^1 + \delta_i^1$, equation (2.70) becomes:

$$\underline{c_i^1} = \beta_i c_i^0 + \frac{1}{(R_d)_i^0}\left[\left(\frac{v_{0x}}{h} + \frac{\alpha}{h^\alpha}D_f\right)\Delta t c_{i-1}^j + \frac{D_f}{h^\alpha}\sum_{k=2}^{i} f_k c_{i-k}^j\right] = \beta_i \delta_i^0 + c_i^1 \tag{2.70}$$

where the factor

$$\beta_i = \frac{1}{(R_d)_i^0}\left[1 + \lambda - \frac{\Delta t}{h}v_{0x} + \frac{\alpha}{h^\alpha}D_f\right] \tag{2.71}$$

So we have$\delta_i^1 = \beta_i \delta_i^0$. That is, the error is magnified by the factorδ_i when the finite difference equation is advanced one time step. After j no time, we can write which is the amplification factor. For the explicit Euler method to be stable,$\delta_i \leq 1$ or

$$\frac{\Delta t v_{0x}}{h} - (\lambda + 1 + R_{d_i}) \leq \frac{\alpha D_f}{h^\alpha} \leq \frac{\Delta t v_{0x}}{h} - (\lambda + 1 - R_{d_i}) \tag{2.72}$$

- **Stability condition for the temporal fractional order derivative**

In this part the equation (2.73) can still be written in the form:

$$c_{i+1}^j = \left(2 + \lambda - \frac{1}{a_3} + \frac{a_2}{a_3}\right)c_i^j - \left(1 + \frac{a_2}{a_3}\right)c_{i-1}^j + \frac{1}{a_3}c_i^{j+1} + \frac{a_1}{a_3}\sum_{k=1}^{j} w_k^\gamma\left[c(x, t_{j+1-k}) - c(x, t_{j-k})\right] \tag{2.73}$$

Suppose that c_0^j is the only term that contains the error, so the perturbed value is $\underline{c_0^j} = c_0^j + \delta_0^j$ This perturbation gives rise to another perturbed valuec_1^j which is $\underline{c_1^j} = c_1^j + \delta_1^j$, then Equation (2.74) becomes:

$$\underline{c_1^j} = m_i c_0^j + \frac{1}{a_3}c_i^{j+1} - \left(1 + \frac{a_2}{a_3}\right)c_{i-1}^j + \frac{a_1}{a_3}\sum_{k=1}^{j} w_k^\gamma\left(c_i^{j+1-k} - c_i^{j-k}\right) = m_i \delta_0^j + c_0^j \tag{2.74}$$

Where the factor $m_i = 2 + \lambda - \frac{1}{a_4} + \frac{a_2}{a_4}$ is the amplification factor associated with the error with $\delta_1^j = m_i \delta_0^j$ when the finite difference of the equation is advanced by a spatial step, for i spatial step, we have . For Euler's method to explain is stable,$|m_i| \leq 1$ which boils down to the following relationship (2.75):

$$\Gamma_{(2-\gamma)} \left(\frac{D_f \Delta t - v_{0x} h^2}{(R_d)_0^j w_0^\gamma} \right) \leq \frac{h^2}{\Delta t^{1+\gamma}} \leq \Gamma_{(2-\gamma)} \left(\frac{3 D_f \Delta t - v_{0x} h^2}{(R_d)_0^j w_0^\gamma} \right) \tag{2.75}$$

2.6 Conclusion

In this chapter, we started with a detailed description of the physical parameters governing the subsurface environment. Then, we proposed the Advection Dispersion Equation (ADE) and Fractional Advection Dispersion Equation (FADE) models associated with the different input and output conditions according to their performance in describing and understanding the level in different soil types. The basic requirement is the power of the resolution methods exploited and the stability study for these different methods namely: the finite difference method, the Runge Kutta method of order four, and the Euler implicit method, based on an approximation of Grunwald-Letnikov and Riemann-Liouville, Caputo.

Chapter III

Results and discussion

3.1 Introduction

The purpose of this chapter is to present the results obtained with the different resolution methods exploited in the previous chapter. This includes the results of the modeling of physical parameters in the first part, the analysis of the impact and performance of some parameters in the retention of pollutants included in the models (ADE) and (FADE) in the second part, and the third part is devoted to the comparison of the model (ADE) and (FADE) followed by their validations with the experimental and analytical results performed by other researchers.

3.2 Behavior of physical parameters in the subsurface environment

In this work we will exploit the values of the parameters of asymptotic dispersivity a(x) and reaction coefficient found experimentally by [18] through a heterogeneous soil in table 1 below

Use the method of fractional derivatives to solve the burgers equation in order to better assess the level of contamination in heterogeneous underground environments

Conduct experimental studies in the underground environment and compare them with the results obtained numerically.

Assess the impact of climate change on the dispersion of contaminants in underground environments using fractional derived models.

The experimental values of the retardation factor parameters generated by the non-linear sorption were exploited in the work of [59], the same data accompanied by the data

Table 3.1

Parameter data of the depth-dependent reaction and asymptotic dispersivity a(x) .

Parameter	valus	symbole	unit
Soil porosity	θ	0.4	cm^3cm^-3
Fluid velocity	v_0	1	m/day
Soil density	ρ	1.2	gcm^-3
adsorption coefficient	k_0	1/3	cm^3/g
transition zone	x_0	0, 10, 20, 40, 80	cm
observation thickness	x	100	cm
observation thickness	a	20	m
observation thickness	b	50	m

used in the work of N. [13] will be exploited in this work, see table 2 below

Table 3.2

Parameter data of retardation factor, dispersion and degradation coefficient parameters .

Parameter	valus	symbole	unit
Soil porosity	θ	0.4	cm^3cm^-3
Fluid velocity	v_0	1	m/day
Soil density	ρ	1.78	gcm^-3
adsorption coefficient	k_0	1/3	cm^3/g
Sorption partition coefcient	k_d	0.345, 0.75	L/g
Sorption exponent	n	0.32;0.7	
Dispersion coefcient	D	4.0	cm^2/day
degradation coefficient	λ	0.001	day

The values of linear and asymptotic time-dependent dispersion coefficient parameters exploited in the work of [58] are presented in Table 3 below will be exploited in this work.

Table 3.3

Parameter data of retardation factor, dispersion and degradation coefficient parameters .

Parameter	valus	parameter	valus
$D_0(MIML)$	$5.89cm^2/min$	$D_0(MIMA)$	$4.51cm^2/min$
$K_L(MIML)$	4500min	$K_A(MIMA)$	200min
D_m	$0cm^2/min$	D_m	$0cm^2/min$

3.2.1 Spatial variation of the asymptotic dispersion function depending on distance

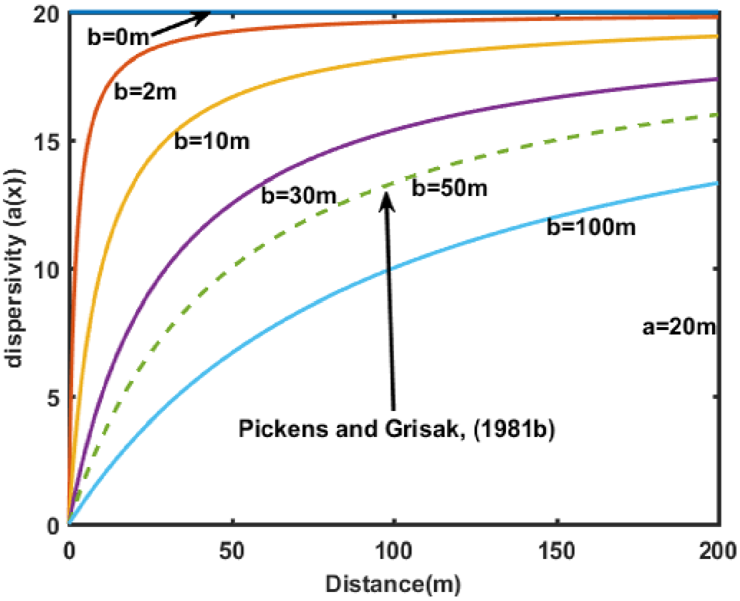

Figure 3.1: Asymptotic dispersion coefficient for various b.

Figure 3.1 shows the spatial variation of the asymptotic distance-dependent dispersivity function for various values of b. The values of b depend on the extent of the pre-asymptotic zone. The smaller the value of b, the faster the dispersivity approaches the asymptotic value. The value of b equal to zero indicates the constant dispersion. The values of b depend on the extent of the pre-asymptotic zone. For a smaller value of b, the dispersivity will approach the asymptotic value faster. A value of b equal to zero indicates constant dispersion.

3.2.2 Time variation of the asymptotic and linear time-dependent dispersion function

Figure 3.2 illustrates the analysis of the asymptotic limit of the time-dependent dispersion coefficient given in relation 2.3, which remains important and more practical in porous media. The values of k depend on the extent of the pre-asymptotic zone. K equal to zero indicates constant dispersion. The smaller the value of k, the closer the dispersion is to the asymptotic value. The values of k different from zero correspond to the times for which the dispersion reaches half of its asymptotic value.

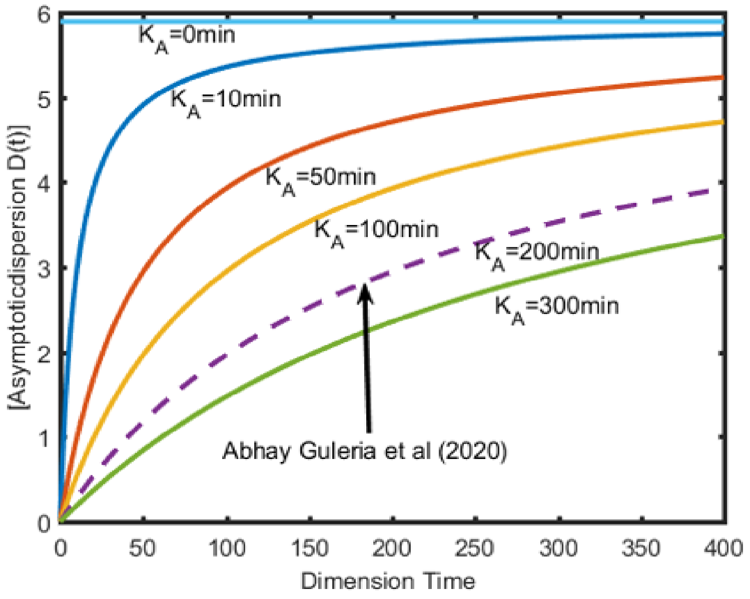

Figure 3.2: Asymptotic dispersion coefficient for various K.

3.2.3 Behavior of the distance-dependent reaction coefficient in subsurface environments

The value of the reaction coefficients decreases faster for a smaller value of x_0 figure 3.3 As x_0 increases from zero to infinity, the shift factors vary between the two special cases of maximum and zero values.

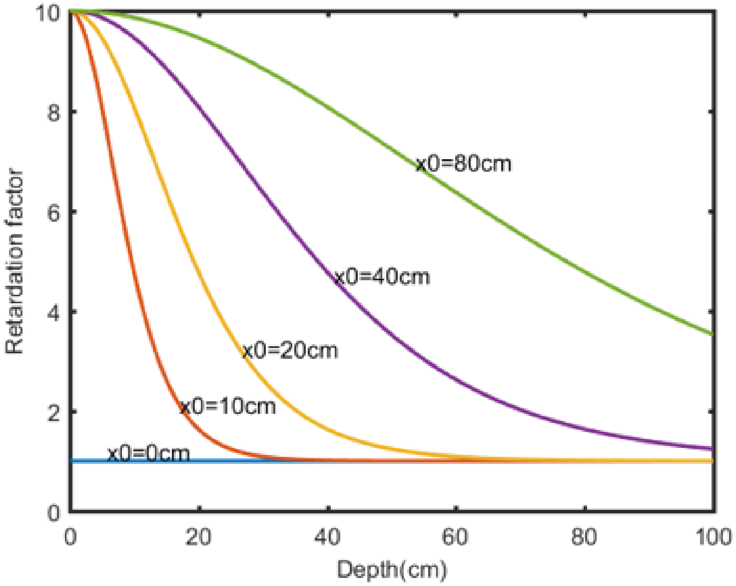

Figure 3.3: The spatial variation of the distance-dependent reaction function for different values of x_0 .

3.3 Solution of the advection-dispersion equation (ADE) with variable dispersion and reaction coefficient

In this section the discretized equation (2.40) associated with the discretized initial and boundary conditions of equation (2.57), (2.58 and (2.59) is simulated to obtain the following results.

3.3.1 Temporal distribution of pollutants in the aquifer and performance of the distance dependent dispersion coefficient with respect to other subsurface parameters

We evaluated the numerical solutions in terms of time, distance, variable dispersion coefficient D (x) and non-variable D, variable absorption coefficient k(x) and non-variable k_d , using model parameters selected in previous studies:ρ_0=1.7 g/l; k0=0.3 cm3/g; $v_0 x$ =1km/year; a=20m; b=50m [1,14,18]. Figure 3.4, b, and c show the relationship between contaminant concentration and time using a constant (a), exponential variable (b), and an initial sinusoidal (c) concentration source. The evaluation of the adsorption rate of pollutants in the aquifer was carried out with an initial concentration of c_0 = 0.6g / l

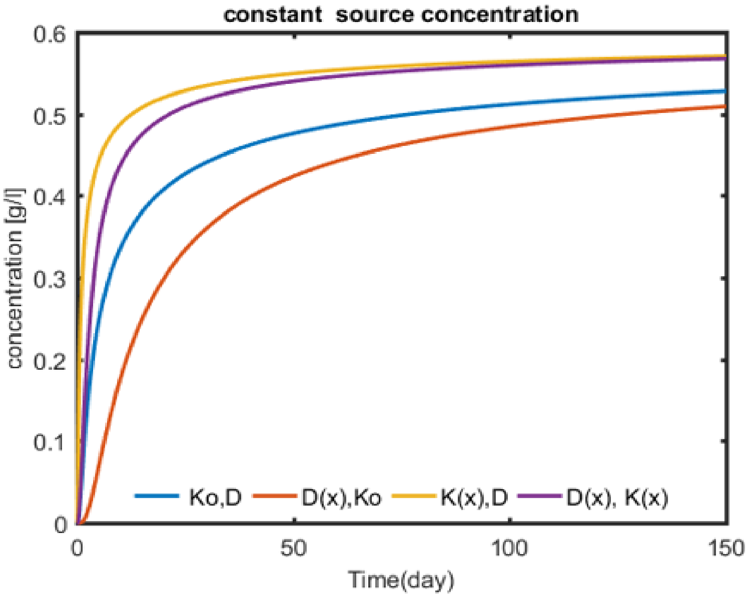

Figure 3.4: Temporal variation of contaminant concentration with constant . c_0 .

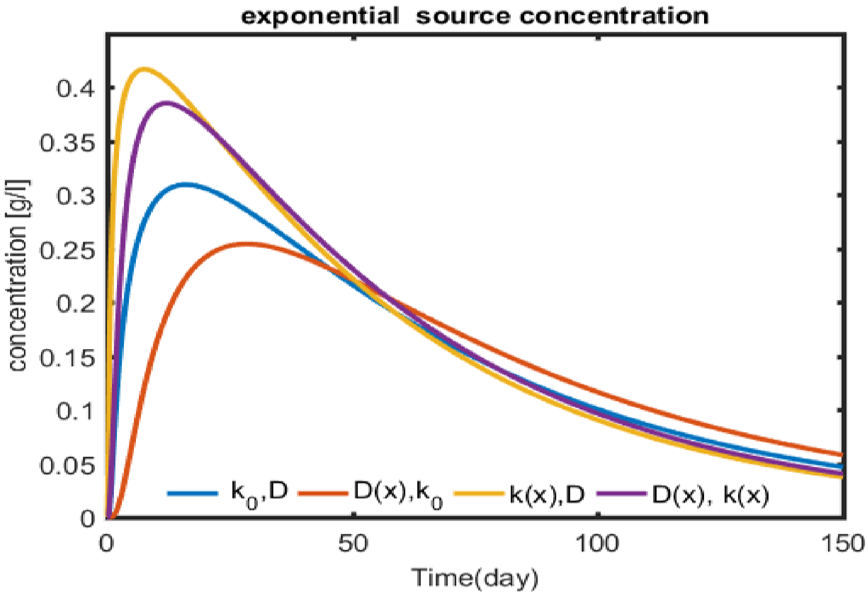

Figure 3.5: Temporal variation of the concentration of contaminants with $c_0$varying exponentially with time.

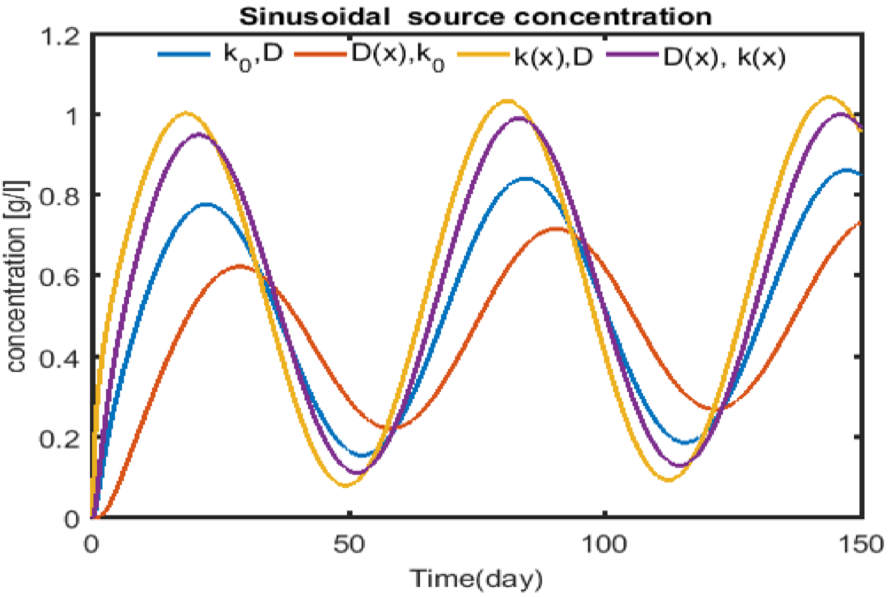

Figure 3.6: Temporal variation of the concentration of contaminants with $c_0$varying sinusoidally with time.

corresponding to the maximum concentration of pollutants taken in the work of cite14. Figure 3.4 compares the temporal distribution of the solute concentration obtained using constant and varying distance-dependent dispersion, constant absorption coefficients, and the distance-dependent variable in the subterranean medium with a constant continuous source at the inlet.

It is observed in figure 3.4, for the case of variable absorption and constant dispersion [k(x), D], that the solute concentration reaches its maximum at c = 0.55g / l in less than 50 days in a water point of the aquifer. On the other hand, the constant absorption and dispersion model depending on the distance [k0, D (x)] reaches its maximum at c = 0.47 g / l in more than 110 days. This is due to the complexity of the distance-dependent dispersion parameters which gives meaning to a good resident time of solutes. This results to low amplitude in the porous medium, in accordance with the work of Gao et al (2013). An interesting observation is that the concentration profiles in all of the above graphs follow an exponential growth pattern of contaminants in the water point of the aquifer. Figure 3.5 compares the temporal distribution of the solute concentration obtained using a constant and distance dependent dispersion variable, a constant and varying distance dependent absorption coefficients in the subterranean medium with a concentration source varying exponentially with time at the entrance of the aquifer. It is observed in figure 3.5 that the solute concentration reaches the first peak at c = 0.417g / l in 50 days and decreases rapidly to a significant minimum at c = 0.041g / l in 150 days at a point d in the aquifer in the case of varying absorption and constant dispersion [k(x), D]. On the other hand, the constant absorption and dispersion model depending on the distance [k0, D (x)] reaches its peak at c = 0.254 g / l in 27.85 days and decreases more slowly to a minimum c = 0.058g / l from 150 days. It is also found that, the models which await the first peaks also return more quickly to their minimum with the smallest concentrations at an increasing time as in the work of [4,13]. The concentration peaks for the [k0, D (x)] are always lower than those of the other models used in this study. The different peaks are due to the fact that the contaminant source has reached the limit which influences the finished system in the aquifer, filled with strong adsorption and degradation.

Figure 3.6 compares the temporal distribution of the concentration of solutes obtained using a constant and variable dispersion model dependent on distance, constant absorption coefficients and variable dependent on distance in the underground medium with a concentration source varying sinusoidally with time at the entrance to the aquifer. This is one of the unusual initial conditions adopted by [13]. It is observed in figure 3.6 that the case of constant absorption and variable dispersion [k0, D (x)] keeps less solute mass unlike at constant dispersion and distance dependent absorption [k(x), D]. The concentrations perform sinusoidal movements with the amplitude of the periodic concentration wave varying throughout the domain according to each model. This is due to the low degree of the nature of the sorption of solutes and natural factors of the subsoil such as temperature, precipitation influencing the subterranean environment. This result is better than those reported in previous studies [4] et de [1] where the advection dispersion equation was considered with constant coefficients as a reference system. The results show that the variable dispersion coefficient and non-variable absorption coefficient [k0, D (x)] strongly influence the transport of pollutants in aquifers compared to the other coefficients studied in this work.

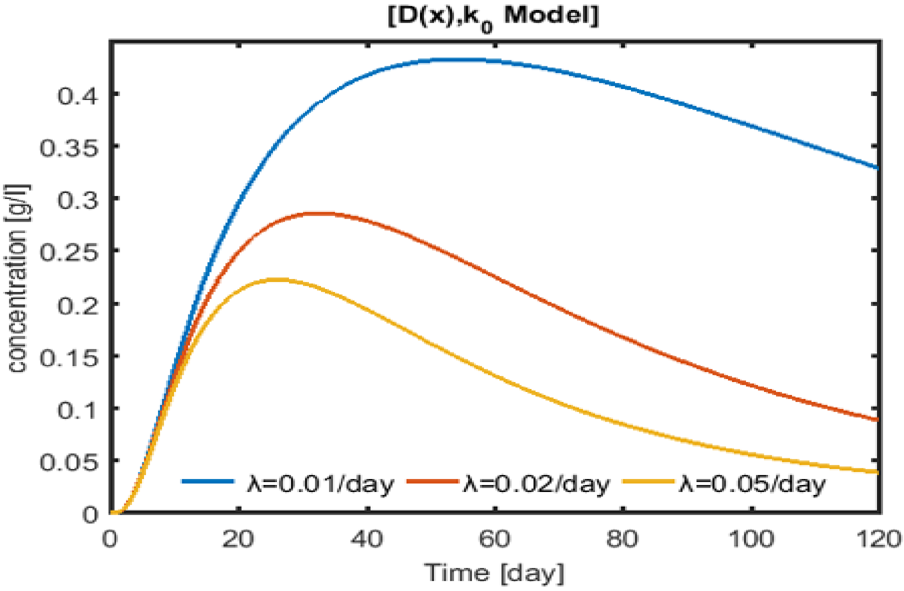

Figure 3.7: Impact of decay constant (*lambda*) on pollutant dispersion considering the aquifer thickness-varying dispersion model and a constant absorption [D(x), ko] with an exponentially time-varying source at the aquifer inlet.

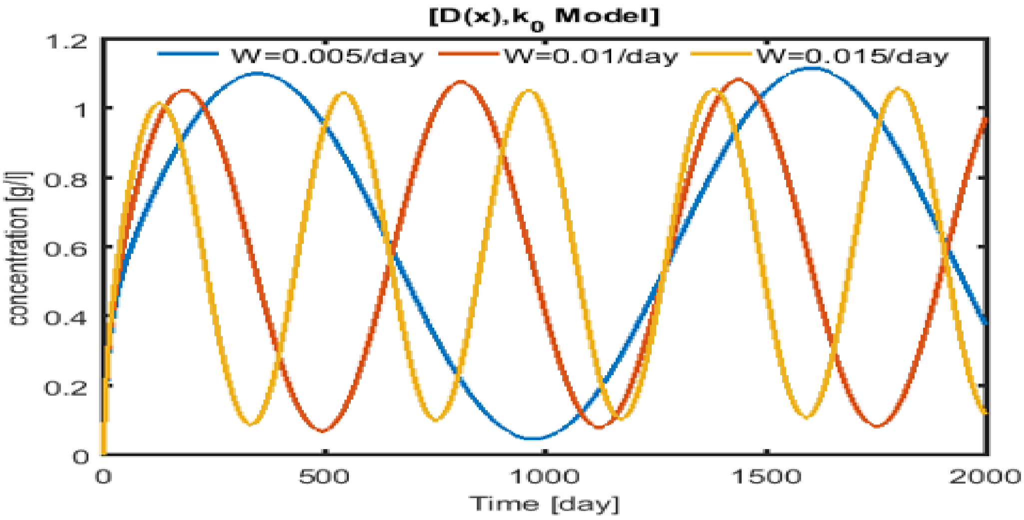

Figure 3.8: Impact of frequency (w) on pollutant dispersion considering the aquifer thickness variable dispersion model and constant absorption [D(x), ko] with a sinusoidally time-varying source at the aquifer inlet.

3.3.2 Influence of frequency (w) and decay constant (λ) on pollutant dispersion in the subsurface environment.

The parametric analysis (w and λ) is realized with the solution of the model of dispersion dependent on the depth and the absorption constant [k0, D(x)]. This is done at a distance of x=500 cm from the pollutants source to study the effects of the initial conditions with respect to time. Figure 3.7 compares the variation of solutes concentration with respect to the different frequencies of the sinusoidal entrance conditions (w = 0,005/day; 0, 01/day et 0,015/day). It establishes the difference between wave fronts with periodic concentration in underground media. The concentration wave amplitudes increase with decreasing w, likewise with the phase shift due to the smaller frequency of the input concentration a. The amplitude of the periodic concentration wave increases slightly with time, which contradicts the results of [4] which proved that the amplitude of the concentration wave does not change with W in his study section. Figure 3.8 compares the evolution of the concentration of the solutes with different constants of decrease of the concentration at the source (λ = 0.01 / day, 0.02 / day and 0.05 / day). The concentrations increase faster at the water point of the aquifer with smaller (λ). In addition, when the concentration is maximum, its arrival time becomes greater with a smaller value (λ). Indeed, the decrease in the source concentration rate is slower under conditions of low λ.

3.4 Solution of the advection-dispersion equation (ADE) with variable dispersion coefficients and importance of parameters a and b.

In this section the discretized equation (2.38) associated with the initial conditions and the discretized limits of equation (2.55) and (2.56) is simulated to obtain the following results.

3.4.1 influence of the parameters a (asymptotic dispersivity) and b (half-length characterizing the mean stroke) in the sub-surface medium.

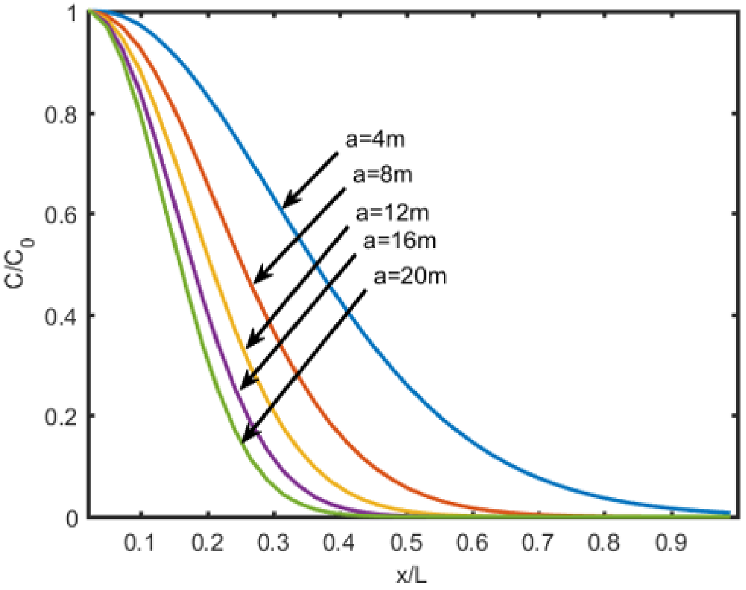

Figure 3.9: Variation of pollutant concentrations in the system as a function of the values of a for b=50m.

The finite differences method was used to evaluate the numerical solutions of the advection-dispersion equation as a function of aquifer length, time, dispersion coefficient varying as a function of distance traveled and the rate of flow of fluids in the aquifer. For this purpose, the model parameters used are presented in Table, were selected in previous studies [4, 13, 52, 88] ; Natarajan., 2015); Al-Niami and Rushton., 1976; corbino, johnny et al., 2016. figure. 3.9 shows the spatial variation of the concentration of pollutants in the porous medium for different values of the dispersivity (a = 4m, 8m, 12m, 16m, 20m) of the dispersion function as a function of depth. Figure. 3.9 also shows that the mass of solute retained in the medium increases with the value of the dispersivity. the concentration profiles follow an exponential decrease in the aquifer independently of the value of the dispersivity a. This result is similar to those of [52]. These authors analytically solved the one-dimensional dispersion advection equation to predict solute transport in heterogeneous porous media with scale-dependent dispersion. It appears that the mass of solute retained in the porous medium increases with the value of dispersivity a. It is also observed that the slope of the concentration profile becomes closer and closer with an increase in a. This is due to the asymptotic variance of the dispersion coefficient which approaches more and more its asymptotic value in the porous medium.

3.4.2 Influence of the different points crossed by the pollutants in the underground environment.

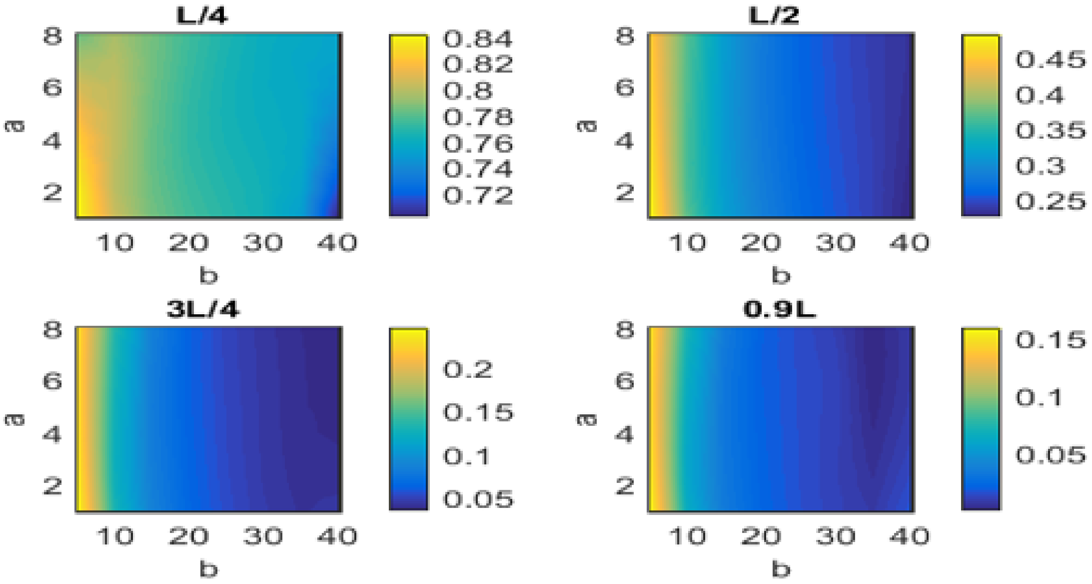

Figure 3.10: Variation of pollutant concentrations in the system as a function of a and b for (t = 50 days, R = 2.5, v = 0.8 m / d).

Four points were selected in the aquifer (L / 4, L / 2, 3L / 4, 0.9L) to evaluate the dispersion behavior of pollutants in the system. Figures 3.10 shows the relationship between the evolution of the pollutant concentration at different points as a function of the dispersion coefficients a and b. The highest values of pollutant concentrations are obtained near the source (x = L / 4) while low values were found near the system outlet (x = 0.9 L). These results show that pollutant dispersion increases with transport distance. The results also suggest that parameter b and a significant effect on pollutant dispersion rather than the asymptotic dispersivity a. For proper environmental modeling of solute transport in porous media, experimental studies should be conducted to find the values of parameters a and b rather than fixing them as done in the literature [4,52] . This result revealed that the adsorption and transport of pollutants in heterogeneous subsurface media are enhanced when the value of parameter b increases. Thus, b has a strong effect on solute transport in the aquifer. However, Darland and Inskeep demonstrated significant effects of pH and temperature on transport through porous columns. Natural phenomena (precipitation and climate change) also influence subsurface parameters [65]

3.5 Numerical solution of Burgers equation associated with time-dependent longitudinal dispersion coefficient.

In this section, the discretized equation (2.47) associated with the discretized initial and boundary conditions of equation (2.60) is simulated to obtain the following results.

3.5.1 Influence of parameters k_A and k_L on the dispersion of pollutants in subsurface media.

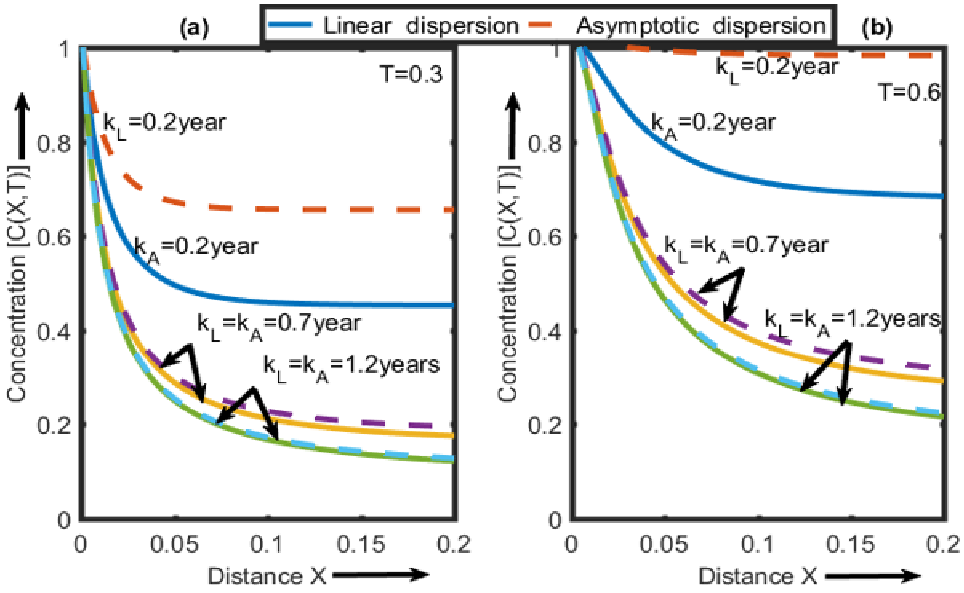

Figure 3.11: Spatial representation of the concentration C (X, T) for de T = 0.3 (a) and T = 0.6 (b) according to the different values of K_L and K_A .

We analyzed the numerical solutions using the following model parameters: C_i=0.01,D_0=0.1 $km^2/year$ λ=0.001 v_0x= 0.01km/year, γ=0.0007 (Das et al., 2017; Guleria et al., 2020

; Natarajan 2016). Figure 3.11a and 3.11b illustrate the spatial and temporal variation in the concentration of the contaminant for different values of K_A andK_L (0.2,0.7,1.2,1.7 years).

Figure 3.11a illustrates the spatial distribution of the concentration of pollutants by considering the different values of$K_L$and K_A. The spatial concentration profiles decrease exponentially in the aquifer for the values of$K_L$and K_A (0.2 years, 0.7 years, and 1.2 years). This profile decreases rapidly when the dispersion function is asymptotic, reflecting greater retention of the mass of solute in the medium. These results are similar to those obtained by [58]. These authors have studied time moments (concentration per unit time) to interpret the behavior of the solute plume in porous media such as porous media laminated hydraulically with a dispersion as a function of time. The different concentrations all decrease together from the entry of the aquifer independently of the dispersion coefficient, to reach horizontal asymptotes at the different positions X = 0.029, 0.054, 0.058 respectively for three values of K_A (0.2 years, 0.7 years, 1.2 years). The percentage of residual concentration associated with these positions is 0.76; 0.30; 0.24. On the other hand, the different horizontal asymptotes are rather obtained at the different positions X = 0.04, 0.055, 0.058 respectively for the values of K_L (K_L= 0.2 years, 0.7 years, 1.2 years). The associated residual concentration percentage is 0.55; 0.28; 0.24. These positions grow with the increase of $K_L$and K_A. The percentage of residual solute concentration remains low when the dispersion function is asymptotic. These results confirm that the increase in K_A assigned to asymptotic time-dependent dispersion coefficients significantly reduces the mass of solute in the subterranean medium compared to K_L associate with linear dispersion coefficients. The concentration profiles in the porous medium approach when the characteristic $K_L$and $K_A$of the medium increase. For the values of$K_L$and K_A<1.2 years, a significant retention of the mass of solute is observed when the dispersion function is asymptotic. A similarity of the concentration profiles is observed for the value of $K_L$and K_A $\leq$1.2 years. This similarity of the concentration profile is due to the temporal variation of the effective dispersion coefficient without upper limit in the underground medium [58].

Figure 3.11b shows that the retention of the mass of solute gradually decreases compared to that observed in Figure 3.11a. Likewise, for the values of $K_L$and K_A<1.2 years, a significant retention of the mass of solute is observed when the dispersion function is asymptotic. Also, an analogy of the concentration profiles is observed for the value of $K_L$and $K_A \leq 1.2$ years.

3.5.2 Impact of molecular diffusion coefficient in subsurface environments.

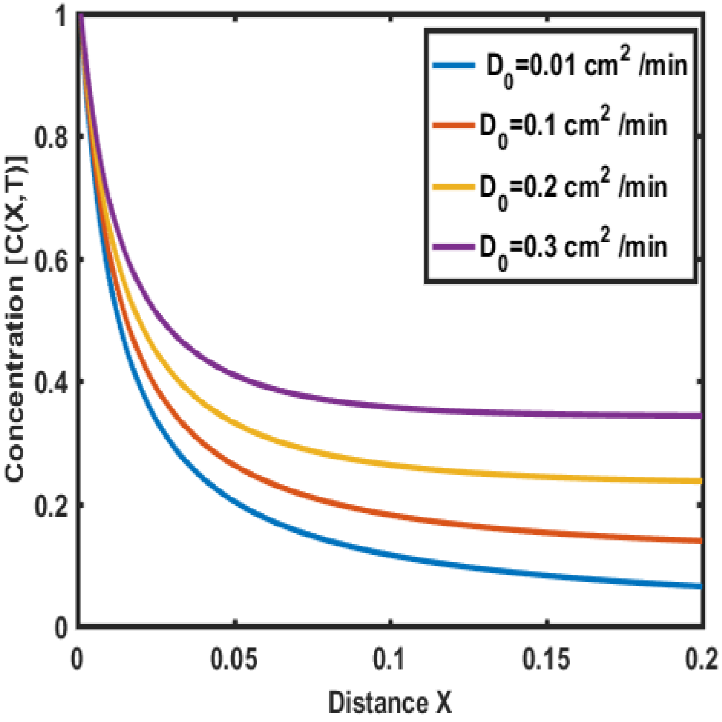

Figure 3.12: Variation of pollutant concentrations in the system as a function of values. .

Figure 3.12 represents the evolution of the pollutant concentration in the space for values of molecular diffusion fixed successively D_0 (0.01, 0.1, 0.2,0.3 . This result reveals that the adsorption of pollutants in subsurface media is improved when the values of molecular diffusion become small in the subsurface media.

3.6 Solution of the fractional order advection-dispersion equation FADE associated with nonlinear adsorption phenomena in subsurface media.

In this section the discretized equation (2.51) associated with the discretized initial and boundary conditions of equation (2.55) and (2.56) is simulated to obtain the following results.

3.6.1 Effect of absorption intensity (n) on the spatial distribution of the concentration of pollutants in a subsurface environment.

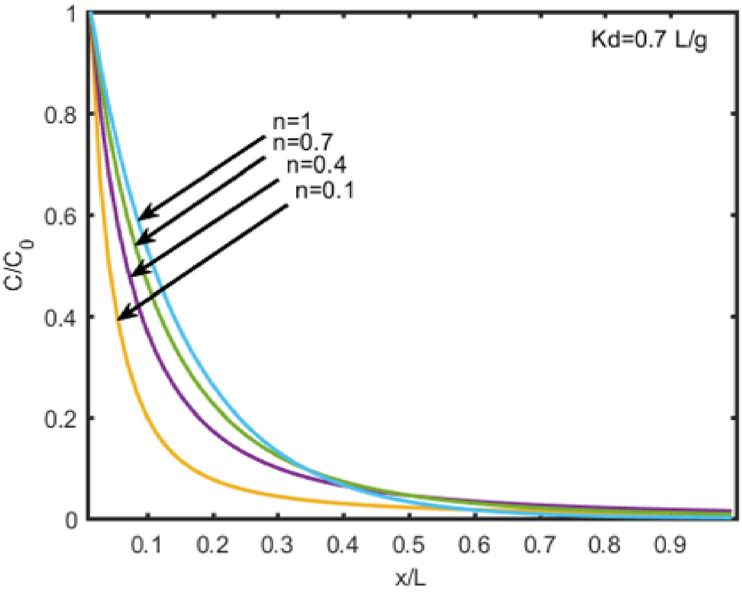

Figure 3.13: Variation of pollutant concentrations in the porous medium as a function of the depth of the medium with the values of absorption intensity (n) fixed for k_d=0.345 L/g, $\alpha = 2$.

Euler's explicit method associated with Grunwald's fractional derivative approximation was used to evaluate the numerical solutions of the advection-dispersion equation as a function of aquifer length, time, constant dispersion coefficient, and flow velocity fluids in the aquifer. For this purpose, the model parameters used, see Table 1, were selected in previous studies cite13,88,89,59 . Figure 3.13 shows the spatial variation of the concentration of pollutants in the porous medium for different values of absorption intensity n (n = .1, 0.4, 0.7, 1) for the absorption coefficient Kd = 0.345 L / g. Figure 3 shows that the mass of solute retained in the subterranean medium increases with the value of n. The concentration profiles follow an exponential decrease in the aquifer regardless of the absorption intensity n. This result is similar to those of Natarajan.,(2020). These authors numerically simulated a mathematical model with four types of input conditions, [13] to assess the variability of the dispersion coefficient on temporal and spatial scales on the mechanism of contaminant transport in saturated porous media. It appears that the mass of solute retained in the porous medium increases with the value of n. It is also observed that the slope of the concentration profile gets closer and closer with a decrease in the value of n. [60] confirm these results by showing that, the retardation coefficient increases non-linearly with decreasing concentration and that the trend is reversed and the retardation factor decreases when n increases above the specific concentration.

3.6.2 Effect of spatial fractional order on the spatial distribution of pollutant concentration in a porous medium.

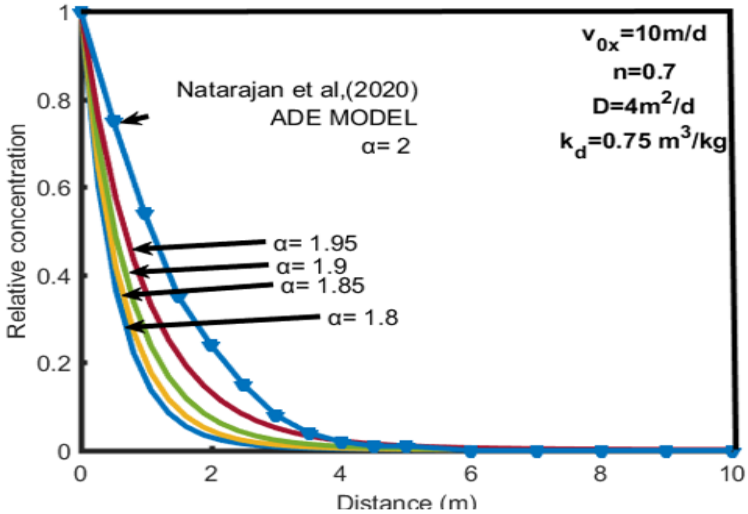

Figure 3.14: Influence of the spatial fractional order (α) on the spatial distribution of the concentration of pollutants in a porous medium comparable to the result produced numerically by [13] through a classical ADE model where α=2

Euler's explicit method associated with Grunwald's fractional derivative approximation was used to simulate the numerical solution of equation (2.51) as a function of aquifer length, time, constant dispersion coefficient, and the flow rate of fluids in the aquifer. For this purpose, the parameters of the model used were selected in previous studies [12, 13, 22, 59]. Figure 3.14 presents the Spatial variation of the concentration of pollutants in the porous medium for different spatial fractional-order values α (α =1.8, 1.85, 1.9, 1.95.2) for the absorption coefficient Kd=0.75 L/g and n=0.7. Figure 3.14 shows that the mass of solute retained in the underground medium increases with (α). The concentration profiles follow an exponential decrease in the aquifer independently of the spatial fractional order (α). This result is similar to those of [13] for the case of the classic ADE model where α=2. These authors numerically simulated a mathematical model with four types of input conditions, to assess the variability of the dispersion coefficient on temporal and spatial scales on the contaminant transport mechanism ants in saturated porous media. They did not take into account the spatial fractional advection-dispersion equation (s-FADE) model, which remains today the most complex model to assess the level of a contaminant in underground environments, which is the object of our work. It is also observed that the slope of the concentration profile becomes closer and closer with a decrease in the value ofα.

3.6.3 Influence of different points (L / 4, L / 2, 3L / 4, 0.9L) on pollutant dispersion using the s-FADE model.

Four points were selected in the aquifer (L/4, L/2, 3L/4, 0.9L) to assess the dispersion behavior of pollutants in the system. Figures 3.15 and 3.16 show the relationship between the evolution of the concentration of pollutants at different points as a function of the absorption coefficients (k_d) and the absorption intensity (n) by successively using the equation model of fractional advection-dispersion (FADE) and the classical advection-dispersion equation (ADE) model. The highest values of pollutant concentrations are obtained near the source (x = L / 4) while the low values were found near the outlet of the system (x = 0.9 L). These results show that the dispersion of pollutants increases with the transport distance. The results also suggest that absorption coefficients (k_d) have a strong effect on pollutant dispersion rather than absorption intensity (n). We observe in

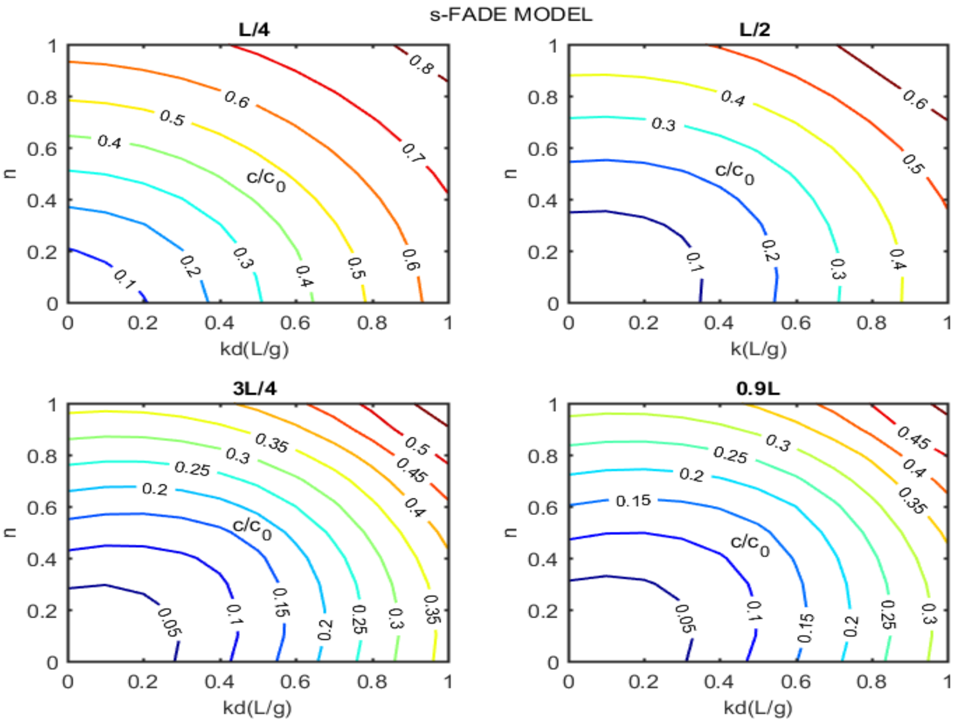

Figure 3.15: Variation of pollutant concentrations in the aquifer system as a function of and n in the porous medium for considering a FADE model at t = 30 days and $v_0x = 1$ m / day, α=1.8.

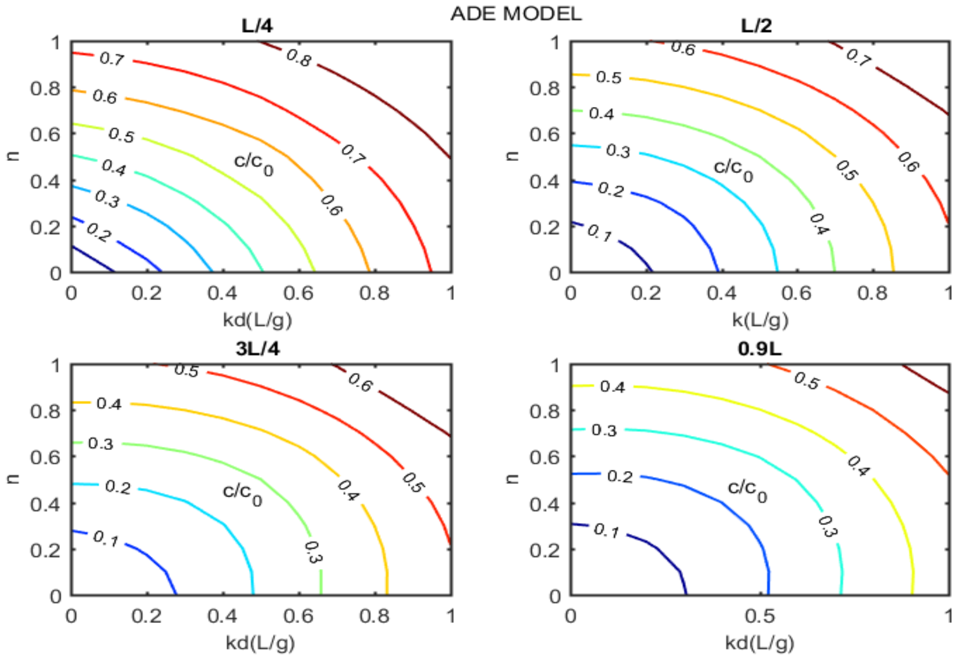

Figure 3.16: Variation of pollutant concentrations in the aquifer system as a function of and n in the porous medium for considering a ADE model at t = 30 days and $v_0 x = 1$ m / day.

figure 3.16 better retention of the concentration of pollutants due to the different degrees of heterogeneity generated by the model (FADE) to explain the process of solute transport in natural porous media. Figures 3.15 and 3.16 give us information on the zones that were exploited by [59] from the entrance to the exit of the aquifer because in their work they took the value k_d =0.345 L/g and n=0.32. [13] meanwhile, he rather set the value k_d =0.75 L/g and n=0.7 which remains localized according to our study in the areas of average concentrations. In the light of Figures 3.15 and 3.16, it emerges that the data of the absorption coefficients k_d and the intensity of absorption n exploited by their work are well located in a precise zone in the aquifer according to the selected points. For proper environmental modeling of solute transport in porous media, experimental studies should be performed. By specifying which point of the aquifer is exploited in relation to the source of the pollutant, to find the values of absorption k_d and the intensity of absorption n, rather than fixing them as is done in the [13] literature. It is also possible to find the range of these parameters that could improve system performance.

3.6.4 Behavior of the pollutants at the aquifer outlet (0.9L) for the FADE model.

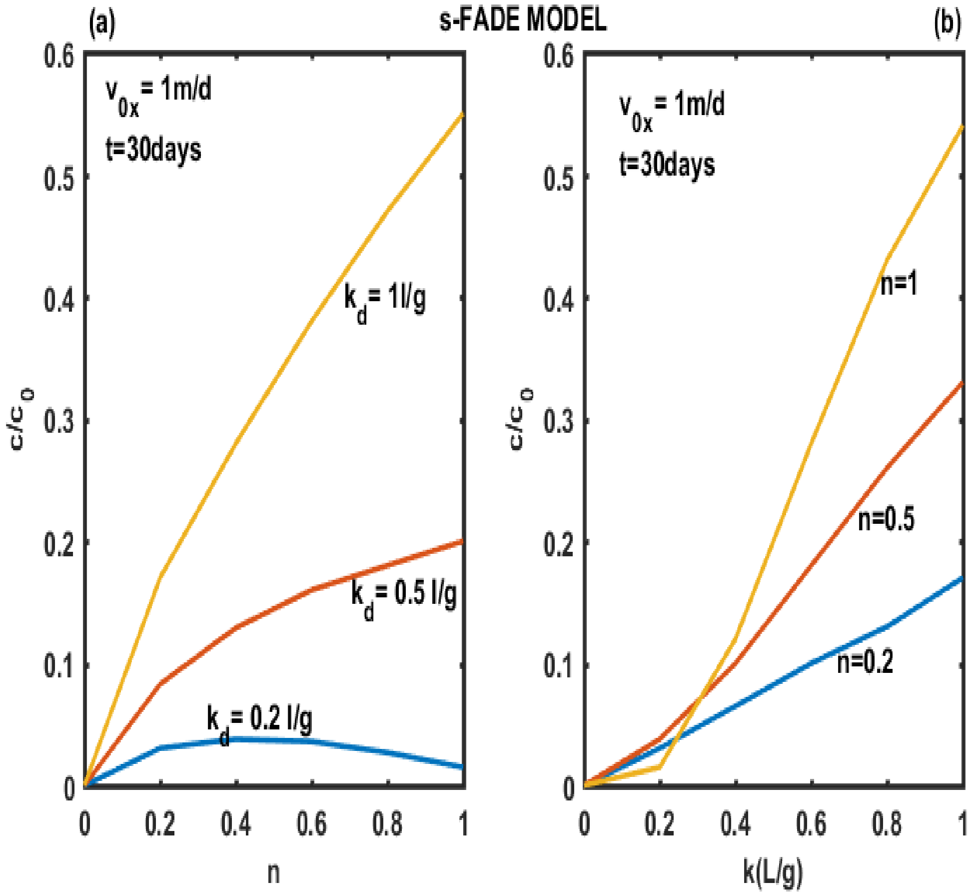

Figure 3.17: behavior of pollutants at the aquifer outlet (0.9L) considering the FADE model at t = 30 days and $v_0x = 1$ m / day.

Figures 3.17 and 3.18 show the evolution of pollutant concentrations as a function of different absorption constants (k_d) and absorption intensity (n) near the aquifer outlet (0.9L) for the two models s-FADE and ADE. These two figures allow us to find the range of these parameters and n which can improve the performance of the system. It has been noted in Figure 3.17 that, for equal to 0.2 L/g and all the values of n $\in R+$ in the aquifer, the lowest concentration values are observed with a range between 0 and 3% of the initial concentration, it has also been noted in Figure 3.18 that, for k_d equal to 1 L/g and all the values of n ?R +, the highest concentration values are observed with a range between 0 and 0.68 of the initial concentration. When analyzing the absorption constants (k_d) and the absorption intensity (n) for the model concentration profiles FADE, it appears that

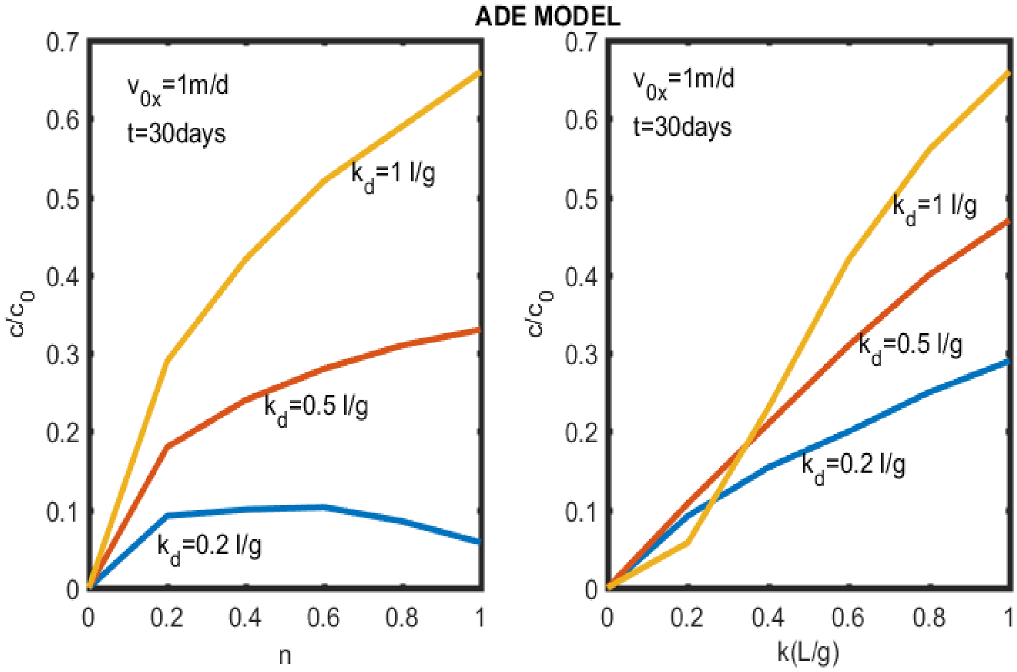

Figure 3.18: Pollutant behavior at the aquifer outlet (0.9L) for a classical dispersion advection equation model at t = 30 days and $v_0x = 1$ m / day .

the appropriate values of Kd are less than or equal to 0.2L/ g for all values of n ∈R+. The high concentration values are obtained for k_d greater than or equal to 1L/g. Figure 3.17 shows that, for (k_d) equal to 1 L/g, the same trend is observed as in Figure 3.17 for the FADE model. However, for k_d equal to 0.2 L/g and all the values of n ∈R + in figure 3.18 for the ADE model, the lowest concentration values are observed with a range between 0 and 10% Co rather than 0 and 3% Co as observed in Figure 3.17. These values of k_d found are used at different points of the aquifer in this work to analyze the effect of the nonlinear absorption coefficient on the transport of contaminants in porous media.

3.6.5 Influence of spatial fractional order on the temporal distribution of pollutant concentration in a porous medium.

The discrete equation (2.51) is exploited to reveal the influence of spatial fractional order on the temporal distribution of solute concentration obtained using a distance-dependent variable dispersion coefficient in the subsurface medium with the different values of α(α=1,1.25,1.5,1.75,2) shown in figure 3.19. It is observed that the solute concentration follows an exponential growth pattern in an aquifer water point regardless of

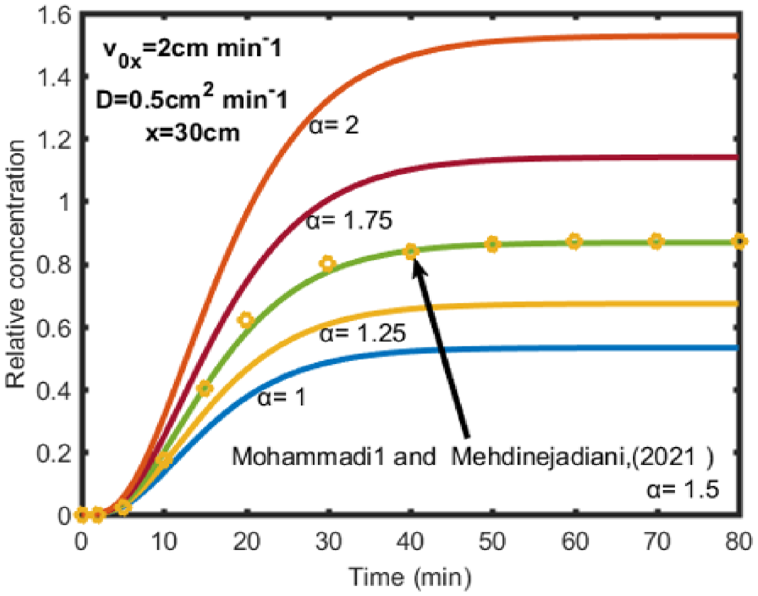

Figure 3.19: Influence of the spatial fractional order (α) on the temporal distribution of the concentration of pollutants in a porous medium comparable to the result produced experimentally by Mohammadi and Mehdinejadiani, (2021) through a s-FADE model with α=1.5.

the value of α. This is in close agreement with the work of [27] who they experimentallyevaluated the impact of the condition at the inlet boundary for α=1.5 in the subsurface medium. Another observed is that the concentration of pollutants increases with the increase of spatial fractional order in a water point of the aquifer.

3.6.6 Influence of temporal fractional order on the spatial distribution of pollutant concentration in a porous medium.

The discretized numerical solution of equation (2.54) associated with the discretized initial and boundary conditions of equation (2.55) and (2.56) is simulated to obtain the results. Figure 3.20 shows the influence of temporal fractional order (γ) on the distribution of solute concentrations in a subterranean medium. The values of the temporal fractional order are chosen in the order γ (γ = 0.2, 0.4, 0.6, 0.8, 1). Figure 3.20 further shows the impact of the absorption coefficient (k_d = 0.2 and 0.75 l/g) on the dispersion of pollutants in the environment. We note that there is low retention of the mass of solute when the value of the time-fractional order (γ) increases in the porous medium and approaches the source of the pollutants when the value of the coefficient of absorption is low in the same medium, which contradicts the work of [26] and Carrer et al, (2019). These authors have developed through the method of boundary elements the solution of the two-dimensional anomalous diffusion equation, and show the ability and necessity of small-time steps to capture the large temporal gradients that arise in the solution of problems governed by ADE containing the fractional derivative. In their work, they did not allude to the parameter of the absorption coefficient k_d which plays the role of possibly causing a solute delay with respect to the mobile fluid in the underground medium. By analyzing these results, it appears that the retention of the mass of solute increases with absorption coefficient k_d. The advection dispersion model becomes classic whenγ=1.

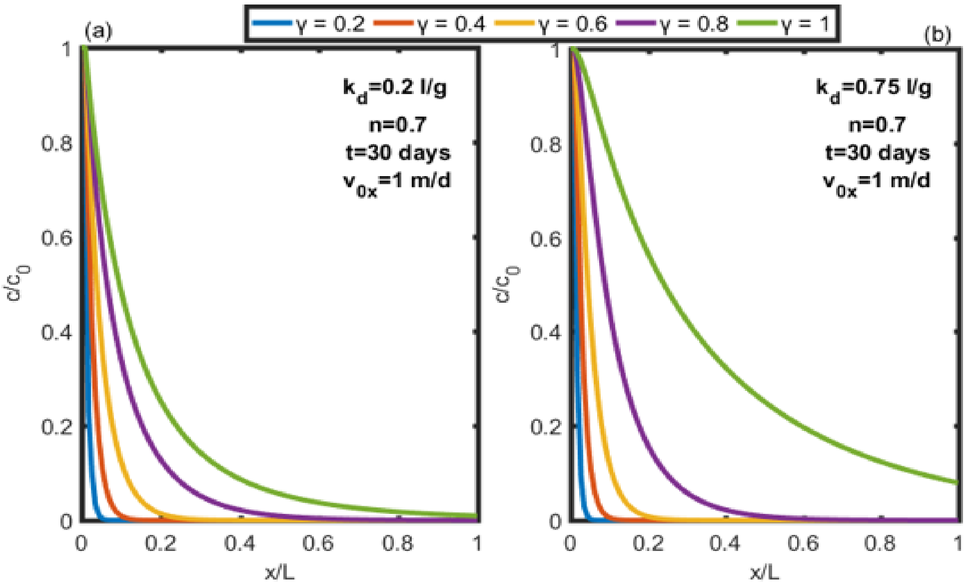

Figure 3.20: Influence of temporal fractional order on the spatial distribution of pollutant concentration in a porous medium.

3.6.7 Comparison between the ADE and FADE model on the distribution of pollutants in subsurface environments.

Figures 3.21a and 3.21b successively illustrate the spatial distribution of the concentration of pollutants with selected constants of the absorption coefficient k_d = 0.2 L/g and k_d =0.5L/g. The concentration profiles according to space decrease exponentially in the aquifer for the values of n (0.1, 0.4, 0.7) for the two models s-FAED and ADE whatever the value of k_d . This profile decreases rapidly for the model FAED, reflecting greater retention of the mass of solute in the medium. These results are similar and more complex to those obtained by [22] because they did not take into account the influence of absorption coefficients (k_d) and absorption intensity (n) in their work. These authors have even an experimental study associated with the model s-FADE to model the conservative solutes, in the end, their results indicate that the best simulation was obtained from the s-FADE model compared to the ADE model. The different concentrations all decrease together from the inlet of the aquifer independently of the model, to reach zero horizontal asymptotes for low absorption coefficients (k_d) figure 3.21a. And horizontal asymptotes at the different positions X = 0.29, 0.6, 0.8 respectively for three values of n (0.2, 0.5, 0.7) for the s-FADE model when k_d =0.5l/g figure 3.21a. The residual concentration percentage associated with these positions is 0.05; 0.08; 0.1. On the other hand, the different horizontal asymptotes are obtained rather at the different positions X = 0.5, 0.65, 0.9 for the ADE model respectively for the same values of n (0.2, 0.5, 0.7). The associated residual concentration percentage is 0.1; 0.14; 0.16. These positions increase with the increase of n. The residual solute concentration percentage remains low for the s-FADE model. These results confirm that the increase in n assigned to the s-FADE models significantly reduce the mass of solute in the underground medium compared to the ADE models. This is hard to the different degrees of heterogeneity engendered by the model FADE to explain the process of solute transport in natural porous media [12].

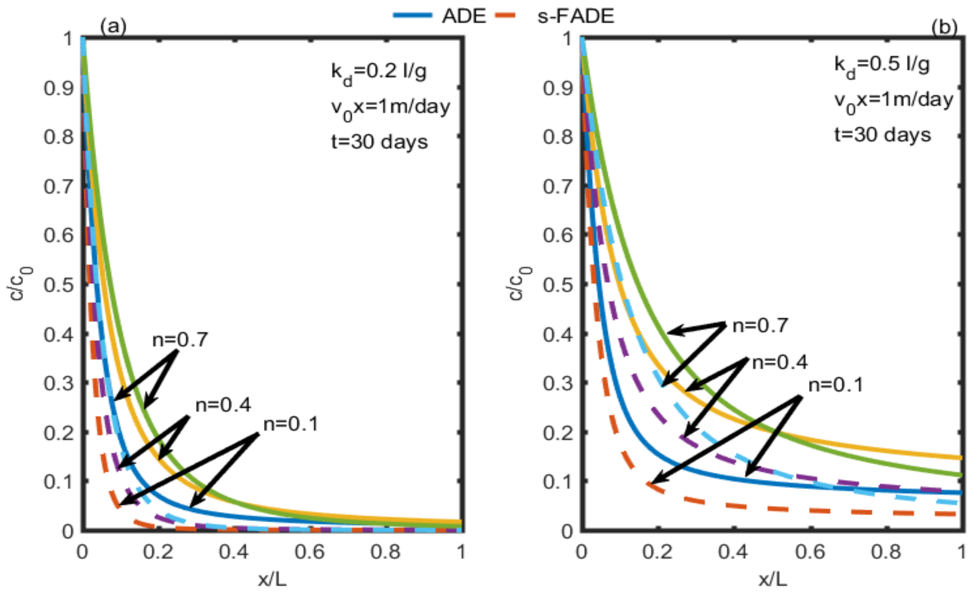

Figure 3.21: Comparison of the pollutant concentration profiles between the s-FADE and ADE model with the values of the parameters n and selected at the aquifer outlet at t = 30 days and $v_0x = 1$ m / day.

3.7 Validations of the models.

3.7.1 Numerical validations of the ADE model with the Analytical solution found by the other researchers.

An analytical solution provided by [91] is used as shown in Figure 3.22 to justify the correct implementation of the model. It is observed from Figure 3.22 that there is a close agreement between the numerical solution and the analytical solution. Therefore, our model can be used to predict the concentration distribution curves as a function of aquifer thickness with different inlet and outlet boundary conditions.

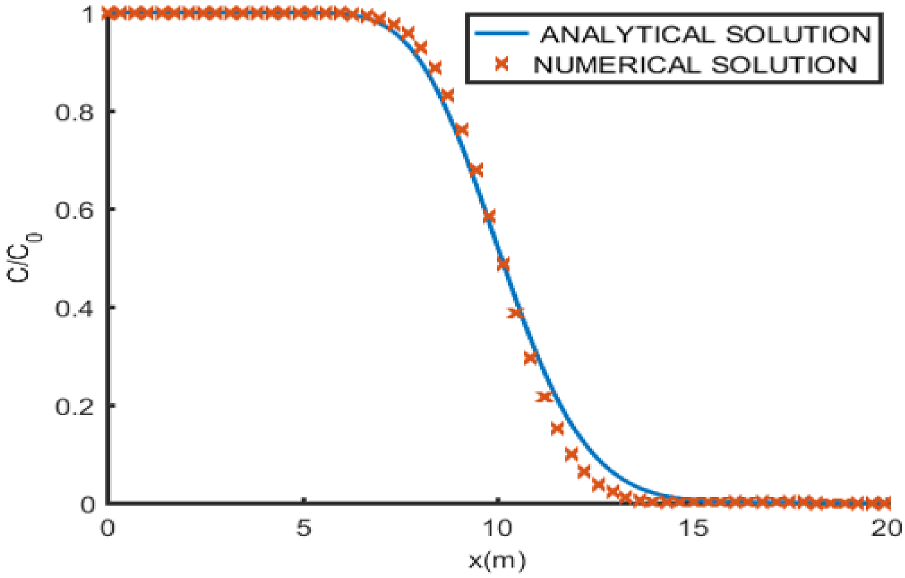

Figure 3.22: Validation of the numerical solution with the analytical solution of the one-dimensional advection-dispersion equation in a homogeneous medium provided by [91]. Parameters used: velocity = 1 m / d; dispersion coefficient = 0.1 m^2 / d; delay factor = 1; total simulation time = 10 days; and domain length = 100 m

3.7.2 Numerical validations of the FADE model with experimental studies found by other researchers.

An Experimental solution on the contaminant transport equation in an underground environment with a constant source of contaminant provided by [27] is used as shown in the Figure (3.23) below. It is observed from figure 3.23 that there is a good agreement between the numerical solution and the experimental solution from the model presented. The latter highlights the use of our model to describe and understand the level of contaminants in porous media.

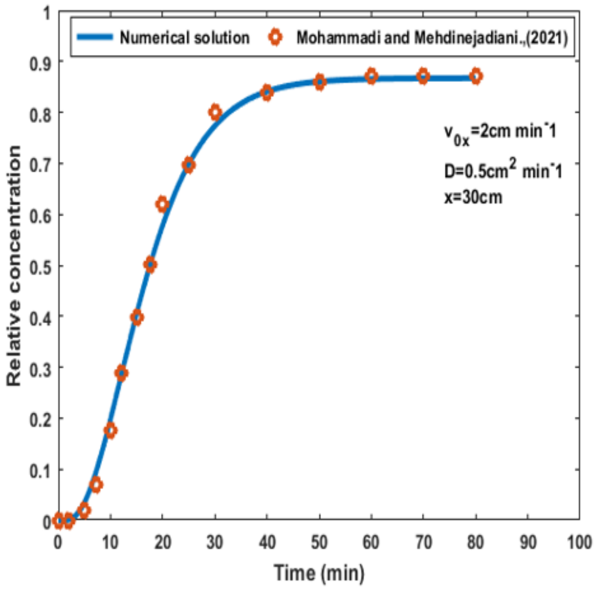

Figure 3.23: Validation of the numerical solution with experimental solution of the contaminant transport equation in an underground environment by [27]. Parameters used: dispersion coefficient =0.5 cm^2/min , fractional order=1.5, total duration of the simulation = 80 min ; and domain length = 30 cm, flow velocity=2cm/min

3.8 Conclusion

In this chapter, we have used the MATLAB programming language to simulate and analyze the behavior of the physical parameters (time and space-dependent dispersion coefficient and the reaction coefficient) in the subsurface environment. Then, to show the importance of the distance-dependent dispersion coefficient concerning the other parameters governing the subsurface environment to evaluate the impact of an (asymptotic dispersivity) and b (half-lengths characterizing the mean course) included in the distance-dependent dispersion coefficient. To study the comparison between the linear and asymptotic time-dependent dispersion coefficient to determine the values of the linear KL and asymptotic KA dispersion parameters, where the concentration profiles of the pollutants converge. Finally, a comparison was made between the (ADE) model and the (FADE) model and it was found that due to the different degrees of heterogeneity generated by the (FADE) model, this model significantly reduces the mass of solute in the subsurface environment compared to the ADE model. The validation of our results justifies a close agreement between the numerical, experimental, and analytical solutions, proving that, our model can predict the concentration distribution curves in the subsurface media.

General Conclusion

Groundwater is recognized as an economic resource and an ecological heritage that is important to manage and preserve. This is more important for a country where water needs (irrigation and industry) are mainly groundwater. The main objective of this research was to aims to determine the location of drinking water points and their consumption times in relation to the source of the pollutants, by evaluating the effect of dispersion and adsorption models of contaminants on the spatio-temporal distribution of pollutants in a porous medium in a groundwater table of finite thickness. Provide a numerical solution of the transport equation by associating the asymptotic function of dispersion and reaction which is a function of the thickness of the aquifer, with three initial conditions of pollutant concentration (constant, exponentially, and sinusoidally variable as a function of time), imposed at the entrance of the aquifer to evaluate the concentration profile of the pollutants in the groundwater environment. Numerically solve the Burgers equation associated with longitudinal time-dependent dispersion phenomena to discuss and determine the dispersion parameters related to the concentration profiles using the two time-dependent dispersion coefficients. To study the concentration profile of the pollutants as a function of the parameters n (sorption intensity or Freundlich parameter) and k_d (adsorption coefficient) on four points taken in the aquifer to select the values of n and Kd at the aquifer outlet using two models (ADE) and (FADE) to optimize the retention of the pollutants in the subsurface environment. The first step of this study focused on the Spatio-temporal distribution of pollutants in the aquifer and show the performance of the distance-dependent dispersion coefficient compared to other subsurface parameters, and also the ability of the asymptotic time-dependent dispersion parameter in the retention of solutes. The one-dimensional advection-dispersion equation is solved numerically by the finite difference method to evaluate the impact of depth-dependent variable dispersion and adsorption coefficient on the retention of pollutants in groundwater. The analysis of the different results obtained reveals that the concentration of pollutants decreases more when the dispersion coefficient is variable and the adsorption coefficient remains non-variable in aquifers compared to the other coefficients studied in this work. It is revealed that as a water point placed in porous medium ages, the dispersion phenomenon in the porous medium tends to better distribute the plume or pollution front in the aquifer. To illustrate the effects of input conditions as a function of time, a parametric analysis was performed under sinusoidal and exponentially decaying input functions. They reveal that the effects of time-dependent input conditions influence the dispersion of pollutants in subsurface media due to the low degree of nature of sorption of solutes and natural subsurface factors influencing the subsurface media. The parameter b (half-length characterizing the mean course) of the distance-dependent dispersion coefficient has a significant impact on the solute movement in saturated porous media compared to parameter an (asymptotic dispersivity). In other words, it has more effect on the dispersion of pollutants in aquifers. The Burgers equation associated with a linear and asymptotic time-dependent dispersion function was also numerically simulated by the Runge Kutta method of order four Rk_4 to determine the Spatio-temporal variation of pollutant concentrations in the subsurface environment. Analysis of the results shows that the concentration profiles decrease rapidly when the dispersion function is asymptotic, reflecting greater retention of solute mass in the subsurface medium. Values of k_L and k_A for which the concentration profiles are similar were determined. These results demonstrate the importance of the nature of the dispersion function on the retention capacity of solutes in the porous medium. In the second step of this study, the solution of the fractional order advection-dispersion equation FADE associated with nonlinear absorption phenomena in subsurface media was applied in the subsurface environment to evaluate its performance compared to the model (ADE). The effect of the delay factor, depending on the nonlinear adsorption on solute transport in porous media was analyzed to understand the importance of adsorption intensity (n), adsorption coefficient (k_d), and spatial and temporal fractional order on the distribution of pollutant concentration in a subsurface medium. The fluency of the different points (L/4, L/2, 3L/4, 0.9L) on the dispersion of pollutants using the FADE model was used to evaluate the behavior of pollutants at the aquifer outlet (0.9L). The explicit Euler method associated with the Grunwald and Caputo-Liousville approximation on fractional derivatives was used to model solute transport. When analyzing the results obtained, the following conclusions were derived from this study: The mass of solute retained in the porous medium increases with the value of n, and the slope of the concentration profile becomes increasingly closer with a decrease in the value of n. The magnitude of the initial concentration of the pollutants is influenced by the different points taken in the aquifer for two dispersion models ADE and FADE used in the aquifer, and thus, the present models project that the resulting mobility of the groundwater contaminant is very sensitive to the aquifer boundary with which it is associated. The sorption partition coefficient (k_d) plays a very significant role in the dispersion of contaminants in the groundwater environment regardless of the model used.

The behavior of the concentration profiles remains the same for the different magnitudes of the absorption intensity(n) throughout the aquifer for both dispersion models. Better retention of solute mass is observed when the model is (FADE) compared to the model (ADE) due to the different degrees of heterogeneity generated by the model (FADE) to explain the solute transport process in natural porous media. The validation of our results justifies a close agreement between the numerical, experimental, and analytical solutions, proving that, our model can describe the profiles and the distribution of contaminants in the underground media. The results of this research display scientific, socio-economic and political interests. Scientifically, this work will provide ecologists, environmentalists, chemists, hydrologists, civil engineers, and thematic modelers with new techniques for modeling and simulating pollutant transport models in subsurface environments to better validate their experimental work. Moreover, our results will be able to show the impacts of the different parameters of the pollutant transport model on groundwater. In terms of socio-economic significance, knowledge of the quality and quantity of water in the groundwater environment will help improve the hygiene and health of the population and prevent major waterborne diseases, both in village communities and in cities. The results of our work will allow the agropastoral and industrial actors of mineral waters to better choose their site of the establishment to improve the output of their companies. At the political level, this study will allow proposing to the local and central decision-makers a reference document for the efficient decision-making on the appropriate sites for the implantation of the drillings and the management of the water resources. This study by its multidisciplinarity and the diversity of its field of application should be sufficiently supported in its realization.

Open problems and future directions

- Use the method of fractional derivatives to solve the burgers equation in order to better assess the level of contamination in heterogeneous underground environments
- Conduct experimental studies in the underground environment and compare them with the results obtained numerically.
- Assess the impact of climate change on the dispersion of contaminants in underground environments using fractional derived models.

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List of publications and conferences

A- Published article

1- **Madie, Y.C**., Togue, K. F., and Woafo, P (2022a): "Analysis of the importance of the dispersion coefficient depending on the distance for the transport of solute in porous media". Springer Sådhanå, 47(2),1-9.

2- **Madie, Y.C**., Togue, K. F., and Woafo, P (2022b): Numerical solution of the Burgers equation associated with the phenomena of longitudinal dispersion depending on time . Elsevier Heliyon, e09776.

3- **Madie, Y.C**., Togue, K. F., and Woafo, P (2022c): Dispersion of pollutants in a porous medium with finite thickness and variable dispersion coefficients. Elsevier Heliyon, e10083.

4- Fulbert togue kamga, Hélé Raïssa Mukam Magne, **Madie, Y.C**, Chamgoue Cheage André, César Mbane Biouele : Modelling Adsorption and Transport of Chrome VI onto Iron Oxide-Coated Sand filter. International Journal of Environment, Agriculture and Biotechnology, 4, 364 (2019) http://dx.doi.org/10.22161/ijeab/4.2.15

B- Posters presentation

- **Madie, Y.C**.,Fulbert Togue Kamga, Woafo P. Modeling saline intrusion in coastal zones.**Hands-On Research in Complex Systems School hold at the Abdus Salam International Centre for Theoretical Physics (ICTP), in Trieste** from 16-27 July 2018.

- **Madie, Y.C**., Togue, K. F., and Woafo, P :Modeling saline intrusion in coastal zones. **6th International conference on Science & Technology of the PK-Fokam Institute of Excellence Yaoundé Cameroon** from 11-13 June 2019.

C- Oral presentations

- **Madie, Y.C**, Fulbert Togue Kamga, Woafo P. Modeling saline intrusion in coastal zones.Hands-On Research in Complex Systems School hold at the Abdus Salam International Centre for Theoretical Physics (ICTP), in Trieste from 16-27 July 2018.
- **Madie, Y.C**,Fulbert Togue Kamga, Woafo P. Modeling saline intrusion in coastal zones. 6th International conference on Science & Technology of the PKFokam Institute of Excellence Yaoundé Cameroon from 11-13 June 2019.
- **Madie, Y.C**, Fulbert Togue Kamga, Woafo P. Numerical simulation of the transport of solutes in porous media with distance-dependent adsorption coefficient: The case of saline intrusion in coastal aquifers. 7th International conference on Science & Technology of the PKFokam Institute of Excellence Yaoundé Cameroon, 26 November 2020.
- **Madie, Y.C**, Fulbert Togue Kamga, Woafo P. Numerical resolution of the equation of the dispersion of pollutants in a porous medium of finite thickness: evaluation of the effect of the parameters and of the boundary conditions. School on Nonlinear and Application; Institute of Mathematics and Physical Science (IMSP), Dangbo Benin from 17-22 May 2021.

D- Conferences

- 6th International conference on Science & Technology of the PKFokam Institute of Excellence Yaoundé Cameroon from 11-13 June 2019.
- 7th International conference on Science & Technology of the PKFokam Institute of Excellence Yaoundé Cameroon from 26 November 2020.

E- Workshops and summer schools

- Hands-On Research in Complex Systems School hold at the Abdus**Salam International Centre for Theoretical Physics (ICTP)** , in Trieste from 16-27 July 2018.

- Professionalization workshop of African scientific journals.**Ministry of scientific research** - October 17, 2019, in Yaounde-Cameroon
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Analysis of the importance of the dispersion coefficient depending on the distance for the transport of solute in porous media

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Abstract. Aquifers are subject to the intrusion of pollutants which may be of natural or anthropogenic origin. This can therefore affect human health through the consumption of borehole water, and also the development of vegetation. However, the natures of the adsorption and dispersion coefficients of the medium significantly influence the retention of pollutants in the underground environment. In this study, the advection dispersion equation is solved numerically to assess the concentration profile of salinity in aquifers for a distance-dependent dispersion coefficient problem. A distance-dependent adsorption coefficient is considered. Analysis of the results shows that the concentration profiles remain very sensitive to the distance-dependent adsorption coefficient. The results obtained show that by considering 0.1g / L of salinity as a guide value in the aquifer and by considering an initial source of pollutant sinusoidally and exponentially varying as a function of time, the necessary time for a drinking water point is prolonged when the dispersion coefficient is dependent on the distance and the adsorption coefficient constant. These results show the importance of measuring these parameters before using them in models.

Keywords. Advection; Dispersal; Drilling; Human health.

1. Introduction

The adsorption of pollutants in porous soils is very important to minimize the risk and vulnerability of aquifers. Today, modeling the transport of solutes in porous media remains a key issue in the fields of soil physics, hydrogeology and environmental sciences, as anthropogenic chemicals frequently enter the soil, subsoil, aquifers and groundwater, whether by accident or through human activities [1]. The resulting chemical residues present risks to the environment and groundwater. These contaminants in groundwater are of industrial origin, household waste, cemeteries, mining debris, and especially contaminants from the sea [1, 2]. Several models and solutions are available to follow the transport of these constituents and most assume that the main transport mechanisms are only dispersed by advection and delay [3]. The rate of adsorption and degradation of solutes is often related to organic soil and mineral content, chemical composition and microbial activity, where organic and mineral content is highly dependent on depth. In general, it has been shown that the contribution of depth to organic and mineral matter is sigmoid in shape [4]. It is interesting to observe the case from a hydrological point of view when the adsorption and dispersion coefficients depend on the depth as the depth increases or decreases the adsorption coefficients can also vary, showing some impacts on the aquifer system. This problem of variable coefficients is likely to be of interest to researchers working on them such as problems of decontamination of groundwater and on aquifer hydrology [5]. Environmental standards limit the concentration of mineral pollutants to 1 to 3 g/ L for surface water and 0.1 g/ L for drinking water [6]. In recent years, several models have been developed by the scientific committee to meet certain objectives. Some examples include, Serrano [7] proposed a solute transport model that takes into account nonlinear adsorption and decay. Coats and Smith [8] developed a conceptual model taking into account dead-end pores in porous media. The concept of the mobile-immobile model (here after referred to as the MIM model) was developed by Van and Wierenga [9] to analyze breakthrough data in aggregate soils. Flury *et al* [10] observed that the spatial variability of the reaction process is generally assumed to be described by a stochastic or deterministic function of space or distance and also experimentally show that the adsorption coefficient decreases sinusoidally with depth.

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*For correspondence

The simulation results developed by Gao *et al* [11] showed that the proposed one-dimensional dispersion advection equation with depth-dependent reaction coefficients was able to capture the evolution of metolachlor concentration at upper soil depths. Xie *et al* [4] proved in their results that the proposed rover-rover model with depth-dependent reaction coefficients was able to satisfactorily capture the evolution of metolachlor concentration both at greater depths and lower. The depth-dependent retardation factor strongly influences the fate and transport of chemicals in the soil. The depth-dependent retardation factor has been validated by Flury *et al* [10] based on a series of experimental data on agricultural soils from various regions of the United States. Experimental data certifies that depth-dependent sorption can cause a bimodal depth profile, even for steady-state water flow. The depth-dependent retardation factor has also been exploited in the work of Xie *et al* [4]. Gao *et al* [11] explored the combined adsorption process in porous media where the adsorption of solutes are related to the content, in organic matter, clay minerals and microbial activity.

An analytical solution of the contaminant transport equation in soils with delay coefficients depending on depth and time dependent entry boundary conditions has been developed by Xie *et al* [4] and Gao *et al* [11] assessed the effects of the depth-dependent delay on the fate and transport behavior of the contaminant in porous media. These authors neglected the impact of the asymptotic dispersion coefficient as a function of the depth in the aquifer as formulated by Abgaze *et al* [12]. In a heterogeneous medium, the pollutant transport equation taking into account a constant dispersion coefficient, becomes questionable to predict the retention of contaminants in aquifers.

Our objective is to provide a numerical solution of the transport equation by associating the asymptotic dispersivity function which is a function of the thickness of the aquifer, with three profiles of initial pollutant concentration conditions which are (a) constant, (b) variable varying exponentially with time and (c) sinusoidally with time. These conditions are applied at the entrance of the aquifer to assess the profile of the concentration of pollutants in underground environments.

2. Materials and methods

2.1 *Physical system*

Figure 1 illustrates the physical system of the problem: the unidirectional horizontal flow of fresh water through an aquifer of finite length L. In this physical system, the dispersion coefficient varies with depth x. This leads to fluctuations in the speed of the fluid, and eventually gives rise to adsorption which increases with distance.

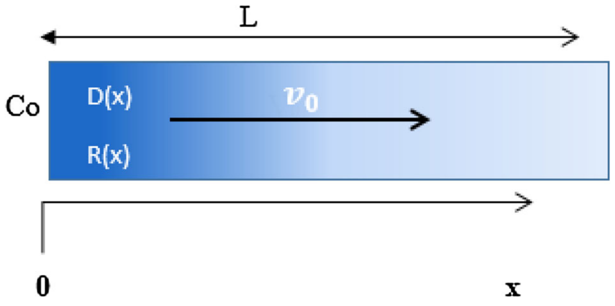

Figure 1. Physical model of the system.

2.2 *Formulation of the mathematical problem*

The inhomogeneity of geological materials caused by irregular stratifications, cracks and faults cause spatially varying hydraulic properties, resulting in fluctuations in fluid velocity, and ultimately result in increasing dispersivity and reaction with increasing frequency of distance. The one-dimensional transport equation of pollutants in the aquifer with variable adsorption and dispersion coefficients is given by the following linear relationship [4, 12]:

$$R(x)\frac{\partial c}{\partial t} = D(x)\frac{\partial^2 c}{\partial x^2} - v_0\frac{\partial c}{\partial x} \tag{1}$$

Where $D(x)$ is the variable coefficient of dispersion as a function of the thickness x with $D(x) = D_0 + \alpha(x)v_0$, with v_0 fluid flow velocity and $R(x) = 1 + \frac{\rho}{\theta}k(x)$ is the retardation factor generated by the variable adsorption coefficient $k(x)$ [4], C the concentration of contaminants.

2.3 *Description of the depth-dependent asymptotic dispersion model*

Dispersion is a physical quantity that occurs when moving away from the injection site, the mass of solute becomes diluted as it moves in the direction of flow (x) to occupy an increasing volume with a corresponding decreasing concentration see figure 2. The description of pollutant transport with a single dispersion parameter becomes inappropriate for predicting the concentrations of contaminants at different distances within a porous medium, therefore, the function of Asymptotic dispersivity as a function of displacement distance is used to embrace the concept of scale-dependent dispersion during solute transport in heterogeneous media [13]

$$D(x) = D_0 + a(1 - \frac{b}{x+b})v_0 \tag{2}$$

Where a is the value of the asymptotic dispersivity (L) which is responsible for the heterogeneity of porous media and it initially increases with the distance traveled and possibly approaching an asymptotic value figure 2, b is

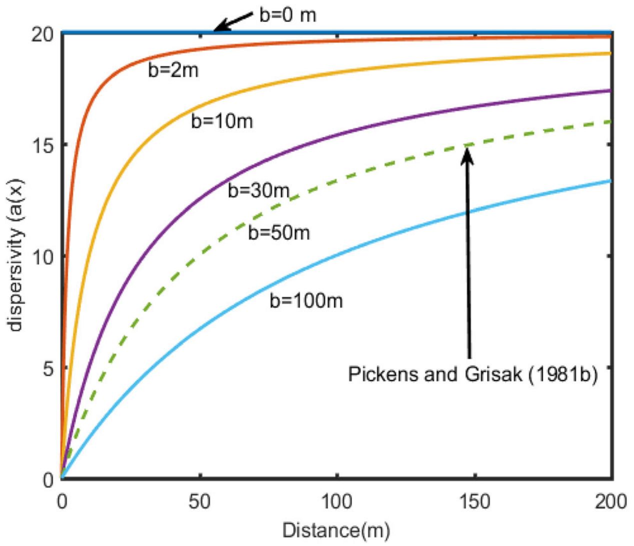

Figure 2. The spatial variation of the distance-dependent asymptotic dispersivity function for different values of b. The values of b depend on the extent of the pre-asymptotic zone. The smaller the value of b, the faster the dispersivity approaches the asymptotic value. The b value equal to zero indicates constant dispersion.

a characteristic distance (L) which determines the displacement distance for dispersivity to reach half of the asymptotic value, D_0 is molecular diffusion and v_0 is fluid flow velocity [12, 13].

2.4 *Description of the variable adsorption model depending on the depth*

As chemicals are transported through the soil, local reaction processes change with depth and differentiate in topsoil and subsoil. We have not yet found a physical consideration for the phenomenon of reaction variation with depth. However, the experimental studies carried out by Flury *et al* [10] based on a series of experimental data on agricultural soils from various regions of the United States showed that the depth distribution of organic matter and microbial activity is sigmoidal in shape. Based on reality observed experimentally by Flury *et al* [10], a depth-dependent reaction function has been adopted below to reflect the combined effects of organic matter and clay minerals on the change in adsorption coefficient with soil depth. The depth distribution of organic matter and microbial activity is sigmoidal in shape. The variable adsorption function is presented as follows [4, 11]:

$$k(x) = k_0 \cosh\left(\frac{x}{x_0}\right) \tag{3}$$

x_0 is a distance between contaminated water and fresh water which determines the rate at which reactions decrease with increasing depth. The depth dependent adsorption function describes the data well, since there is only one adjustable parameter, namely the depth x_0 transition. The value of the reaction coefficients decreases faster for a smaller value of x_0 figure 3. As x_0 increases from zero to infinity, the shift factors vary between the two special cases of maximum and zero values [4]. k_0 is the adsorption coefficient in the topsoil, representing the maximum of k(x).

The values of the depth-dependent reaction parameters R (x) were determined experimentally by Flury *et al* [10]. The values of the parameters of the asymptotic dispersivity a (x) were also given experimentally by Pickens and Grisak [13] through a heterogeneous soil in the table below (Table 1):

2.5 *Initial conditions and limits*

The initial condition constants (a), variables exponentially with time (b) and sinusoidally with time (c) were introduced at the inlet of the aquifer (initial injection concentration). The problem can be defined mathematically by eq. (1) with the following initial conditions and boundary conditions [11]

$$\begin{cases} c(L,0) = 0; \quad for\, 0 < x < L \\ c(0,t) = C_0 \quad for\, all\, t \\ \dfrac{\partial c(L,t)}{\partial x} = 0; 0 < x < L \end{cases} \tag{4}$$

$$\begin{cases} c(L,0) = 0; \quad for\, 0 < x < L \\ c(0,t) = c_0 e^{-\lambda t} \quad for\, all\, t \\ \dfrac{\partial c(L,t)}{\partial x} = 0; 0 < x < L \end{cases} \tag{5}$$

Where λ is the first order decay coefficient. The decay coefficient can be related to the half-life $t_{1/2}$ of a decomposing material.

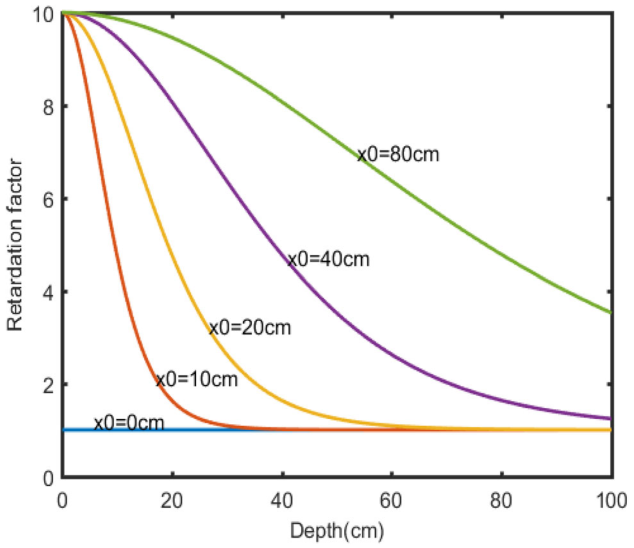

Figure 3. The spatial variation of the distance-dependent reaction function for different values of x_0.

Table 1. Parameters used for simulating concentration profiles.

Parameter description	Symbol	Value	Unity
Soil porosity	θ	0.4	-
Fluid velocity	v_0	1.0	m/day
Soil density	ρ_s	1.2	g/cm^{-3}
Adsorption coefficient in the topsoil	k_0	1/3	cm^3/g
Transition zone	x_0	0, 10,20, 40, 80	cm
Observation thickness	x	100	cm
Asymptotic dispersivity constant	a	20	m
Characteristic distance	b	50	m

The original periodic entry condition is assumed. This condition was chosen experimentally by Ebach and White [14] where the considered concentration at the entrance of the porous medium as the response of a harmonic function of time. The technical frequency response required the response to a sinusoidally varying input concentration. This is one of the unusual initial conditions adopted by Natarajan *et al* [15]. The sinusoidal input shape was used to assess the behavior of pollutants in porous media as reported in previous research [3, 11]. The initial and limiting conditions considered are given as follows:

$$\begin{cases} c(L,0) = 0; \quad for\, 0 < x < L \\ c(0,t) = C_0[1+\sin(wt)] \quad for\, all\, t \\ \dfrac{\partial c(L,t)}{\partial x} = 0; 0 < x < L \end{cases} \tag{6}$$

Where w is the pulsation differentiates the periodic wave fronts. This parameter was also exploited in the work of Gao *et al* [11] to study the effects of time-dependent entry boundary condition.

2.6 *Numerical solution of the mathematical model*

The derivatives of the advection dispersion equation (1) are approximated by the truncated expansion of the numerical centered finite difference approximation scheme to determine the first and second order spatial derivatives are given according to the relation [15]:

$$\frac{\partial c}{\partial x} = \frac{c_i^j - c_{i-1}^j}{\Delta x} \tag{7}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{\Delta x^2} \tag{8}$$

The first order temporal discretization is given by the following relation:

$$\frac{\partial c}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t} \tag{9}$$

The indices (i) and (j) indicate the nodes of discretization along (x) and (t) respectively. Δx and Δt are respectively the spatial and temporal steps. Thus, equation (1) can be written in the discrete form below:

$$C_i^{j+1} - c_i^j = \frac{D_i\Delta t}{R_i\Delta x^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) - \frac{v_{0\Delta t}}{R_i\Delta x}\left(c_i^j - c_{i-1}^j\right) \tag{10}$$

$$C_i^{j+1} = (1 - 2\propto -\beta)c_i^j + \propto c_{i+1}^j + (\propto +\beta)c_{i-1}^j \tag{11}$$

The discretization of boundary and initial conditions is necessary to apply this method. The discrete version of the initial and boundary conditions associated with the equation is expressed as:

$$\begin{cases} c_i^0 = 0, \quad if \quad 0 < i < Nx \\ c_0^j = c_0, \quad if\, j \quad \geq 0 \\ \dfrac{\partial c_{Nx}^j}{\partial x} = 0, \quad if\, j \quad \geq 0 \end{cases} \tag{12}$$

$$\begin{cases} c_i^0 = 0, \quad if\ 0 < i < Nx \\ c_0^j = c_0 e^{-\lambda t_j} \quad for\, all\, t \\ \dfrac{\partial c_{Nx}^j}{\partial x} = 0, \quad if\, j \geq 0 \end{cases} \tag{13}$$

$$\begin{cases} c_i^0 = 0, \quad if\ 0 < i < Nx \\ c_0^j = C_0[1 + sin(wt_j)] \quad for\, all\, t \\ \dfrac{\partial c_{Nx}^j}{\partial x} = 0, \quad if\, j \geq 0 \end{cases} \tag{14}$$

2.7 *The stability condition*

$$\begin{cases} 0 \leq 1 - 2\propto -\beta \leq 1 \\ 0 \leq \propto \leq 1 \\ 0 \leq \propto + \beta \leq 1 \end{cases} \tag{15}$$

Avec $\propto = \frac{D_i\Delta t}{R_i\Delta x^2}$, et $\beta = \frac{v_{0\Delta t}}{R_i\Delta x}$

Then the new solution is a convex combination of the previous equation (15):

$$\begin{cases} \beta \leq 1 - 2\propto \leq 1 + \beta \\ 0 \leq \propto \leq 1 \\ -\propto \leq \beta \leq 1 - \propto \end{cases} \tag{16}$$

Therefore $-\propto\ \leq \beta \leq 1 - 2\propto$

Thus, the conditions of stability are $0 \leq\ \propto\ \leq 1$ and $-\propto\ \leq \beta \leq 1 - 2\propto$

In this work $0 \leq \frac{D_i \Delta t}{R_i \Delta x^2} \leq 1$ and $-\frac{D_i \Delta t}{R_i \Delta x^2} \leq \frac{v_{0\Delta t}}{R_i \Delta x} \leq 1 - 2\frac{D_i \Delta t}{R_i \Delta x^2}$

3. Results and discussion

3.1 *Variation of pollutants concentrations in the system*

We evaluated the numerical solutions in terms of time, distance, variable dispersion coefficient D (x) and non-variable D, variable adsorption coefficient k(x) and non-variable k_0, using model parameters selected in previous studies: ρ_s = 1.7 g/l; k_0 = 0.3 cm^3/g; v_0 = 1 km/an ; a = 20 m; b = 50 m [4, 12, 13]. Figures 4a, b and c show the relationship between contaminant concentration and time using a constant (a), exponential variable (b), and an initial sinusoidal (c) concentration source. The evaluation of the adsorption rate of pollutants in the aquifer was carried out with an initial concentration Co = 0.6g / l corresponding to the maximum concentration of pollutants taken in the work of Abgaze *et al* [12]. Figure 4a compares the temporal distribution of the solute concentration obtained using constant and varying distance-dependent dispersion, constant adsorption coefficients and the distance-dependent variable in the subterranean medium with a constant continuous source at the inlet.

It is observed in figure 4a that for the case of variable adsorption and constant dispersion [k(x), D], that the solute concentration reaches its maximum at c = 0.55g / l in less than 50 days in a water point of the aquifer. On the other hand, the constant adsorption and dispersion model depending on the distance [k_0, D (x)] reaches its maximum at c = 0.47 g / l in more than 110 days. This is due to the complexity of the distance-dependent dispersion parameters which gives meaning to a good resident time of solutes. This results to a low amplitude in the porous medium, in accordance with the work of Gao *et al* [11]. An interesting observation is that the concentration profiles in all of the above graphs follow an exponential growth pattern of contaminants in the water point of the aquifer. Figure 4b compares the temporal distribution of the solute concentration obtained using a constant and distance dependent dispersion variable, a constant and varying distance dependent adsorption coefficients in the subterranean medium with a concentration source varying exponentially with time at the entrance of the aquifer. It is observed in figure 4b that the solute concentration reaches the first peak at c = 0.417g / l in 50 days and decreases rapidly to a significant minimum at c = 0.041g / l in 150 days at a point d in the aquifer in the case of varying adsorption and constant dispersion [k(x), D]. On the other hand, the constant adsorption and dispersion model depending on the distance [k_0, D (x)] reaches its peak at c = 0.254 g / l in 27.85 days and decreases more slowly to a minimum c = 0.058g / l from 150 days. It is also found that the models which await the first peaks also return more quickly to their minimum with the smallest concentrations at an increasing time as in the work of Gao *et al* [11] and Natarajan *et al* [15]. The concentration peaks for the [k_0, D (x)] are always lower than those of the other models used in this study. The different peaks are due to the fact that the contaminant source has reached the limit which influences the finished system in the aquifer, filled with strong adsorption and degradation.

Figure 4c compares the temporal distribution of the concentration of solutes obtained using a constant and variable dispersion model dependent on distance, constant adsorption coefficients and variable dependent on distance in the underground medium with a concentration source varying sinusoidally with time at the entrance to the aquifer. This is one of the unusual initial conditions adopted by Natarajan *et al* [15]. It is observed in figure 4c that the case of constant adsorption and variable dispersion [k_0, D (x)] keeps less solute mass unlike at constant dispersion and distance dependent adsorption [k(x), D]. The concentrations perform sinusoidal movements with the amplitude of the periodic concentration wave varying throughout the domain according to each model. This is due to the low degree of the nature of the sorption of solutes and natural factors of the subsoil such as temperature, precipitation influencing the subterranean environment. This result is better than those reported in previous studies [4, 11] where the advection dispersion equation was considered with constant coefficients as a reference system. The results show that the variable dispersion coefficient and non-variable adsorption coefficient [k_0, D (x)] strongly influence the transport of pollutants in aquifers compared to the other coefficients studied in this work.

The parametric analysis (w and λ) is realized with the solution of the model of dispersion dependent on the depth and the adsorption constant [k_0, D(x)]. This is done at a distance of x=500 cm from the pollutants source to study the effects of the initial conditions with respect to time. Figure 5a compares the variation of solutes concentration with respect to the different frequencies of the sinusoidal entrance conditions (w = 0,005/day; 0, 01/day et 0,015/day). It establishes the difference between wave fronts with periodic concentration in underground media. The concentration wave amplitudes increase with decreasing w, likewise with the phase shift due to the smaller frequency of the input concentration a. The amplitude of the periodic concentration wave increases slightly with time, which contradicts the results of Gao *et al* [11] which proved that the amplitude of the concentration wave does not change with W in his study section. Figure 5b compares the evolution of the concentration of the solutes with different constants of decrease of the concentration at the

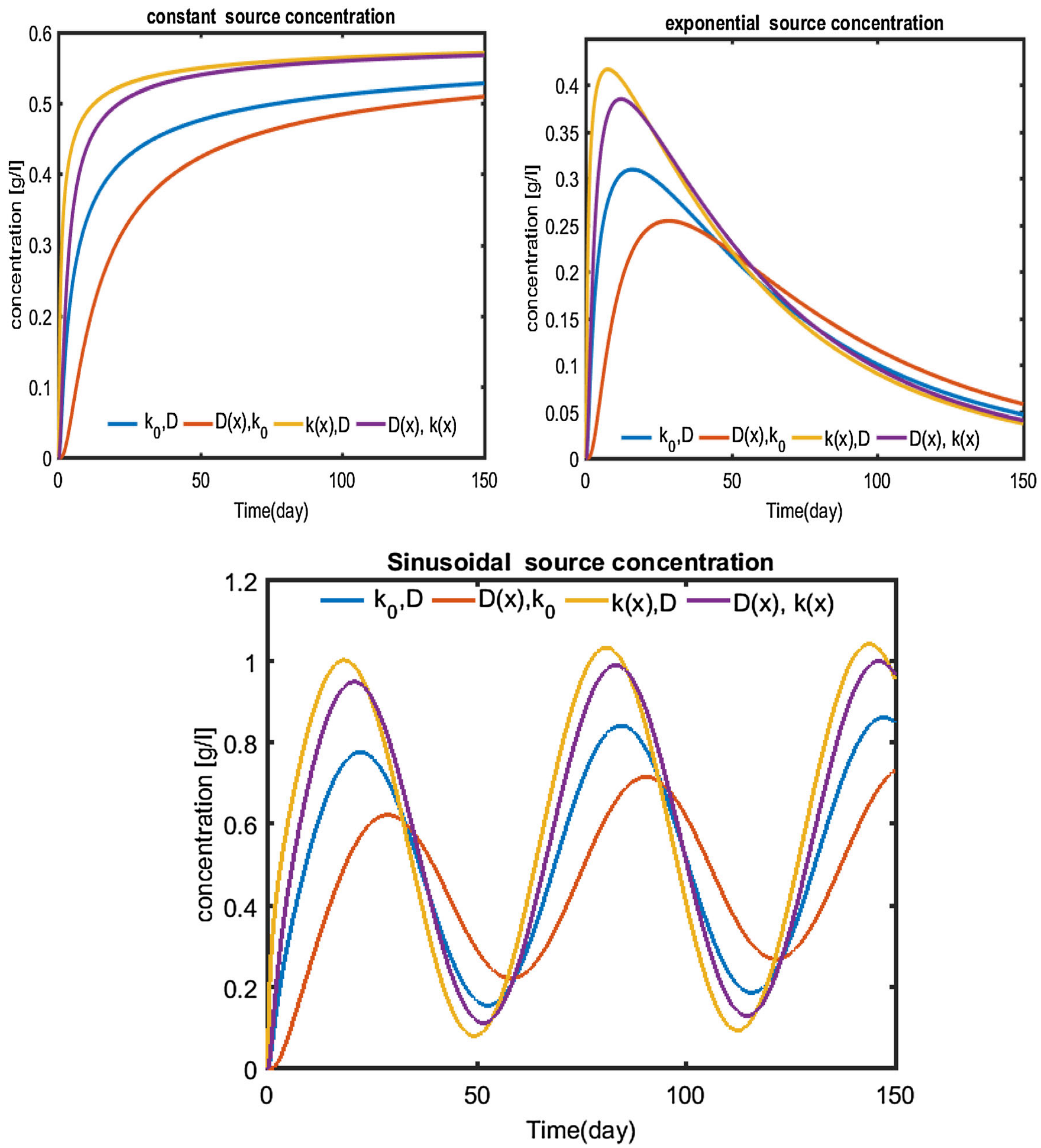

Figure 4. Concentration variation as a function of time with a constant Co (a), varying exponentially (b) and sinusoidally (c) as a function of time.

source (λ = 0.01 / day, 0.02 / day and 0.05 / day). The concentrations increase faster at the water point of the aquifer with smaller (λ). In addition, when the concentration is maximum, its arrival time becomes greater with a smaller value (λ). Indeed, the decrease in the source concentration rate is slower under conditions of low λ.

3.2 *Validation of the model*

An analytical solution provided by Pickens and Grisak [13] using the discrete dispersivity a = 5 cm, is used as shown in figure 6 to justify the correct implementation of the model. It is observed from figure 6 that there exists a close approximation between the numerical solution and the analytical solution. Therefore, our model can be used to predict the distribution curves of the concentrations as a function of the thickness of the aquifer with different conditions at the inlet and outlet limits.

4. Conclusion

This paper proposes the numerical resolution by the method of Runge Kutta fourth order of the one-dimensional advection-dispersion equation, which makes it possible to

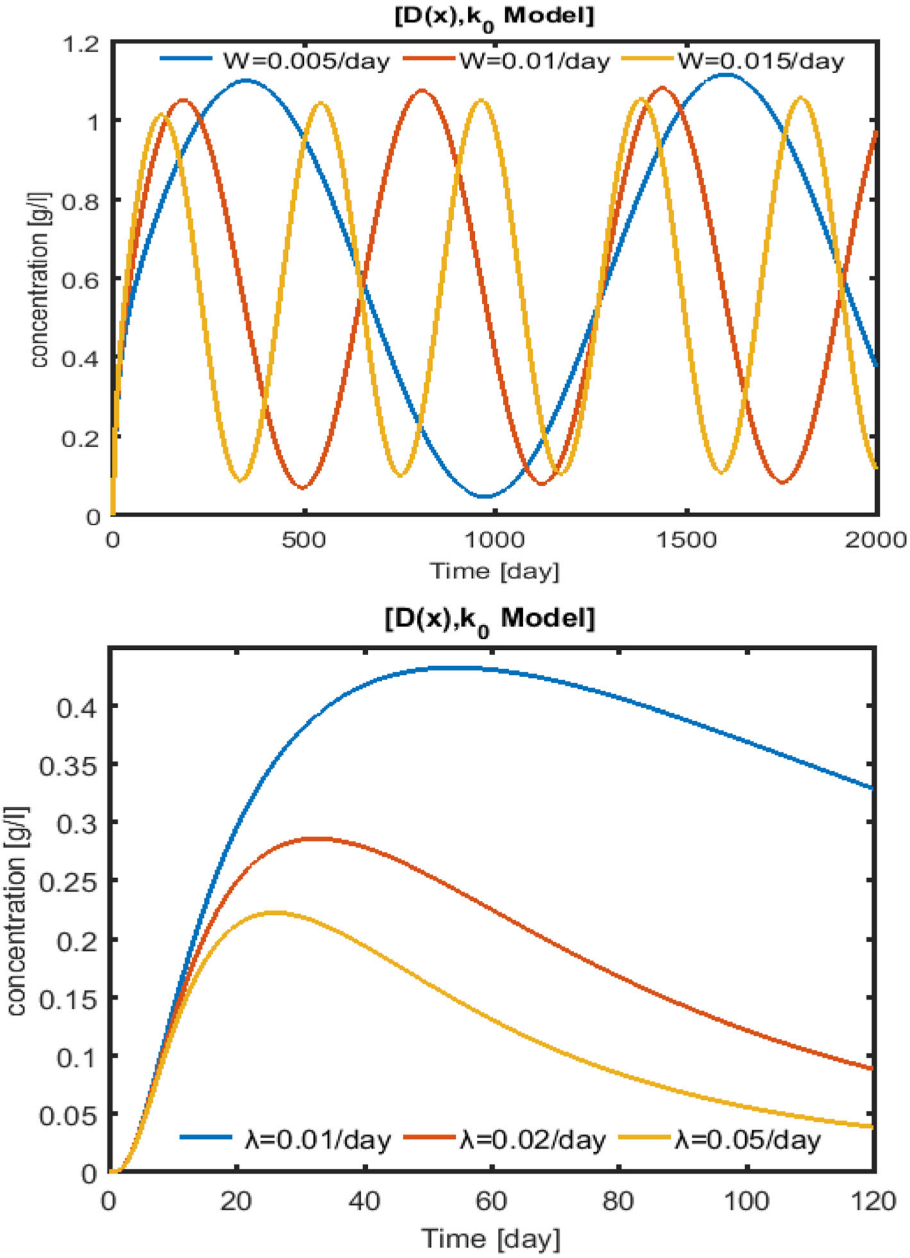

Figure 5. Impact of the frequency (w) and the decay constant (λ) on the dispersion of pollutants by considering the varying dispersion model as a function of the thickness of the aquifer and a constant adsorption [D (x), k_0] with a variable source sinusoidally (a) and exponentially (b) with time at the entrance to the aquifer.

evaluate the impact of the coefficient of dispersion and variable adsorption depending on the depth of the pollutants retained in groundwater. Analysis of the various results obtained reveals that the concentration of pollutants decreases more when the dispersion coefficient is distance-dependent and the adsorption coefficient remains constant [D (x), k_0] in aquifers compared to other cases studied in this work. The more a water point placed in a porous medium ages, the more the phenomenon of dispersion in the porous medium tends to better distribute the plume or the pollution front in the aquifer. To illustrate the effects of input conditions as a function of time, a parametric analysis was performed under sinusoidal and exponentially decaying input functions. They reveal that the time-dependent effects of outlet conditions totally disperse pollutants into subterranean media due to the low degree of solute sorption nature and natural subsoil factors influencing the subterranean environment.

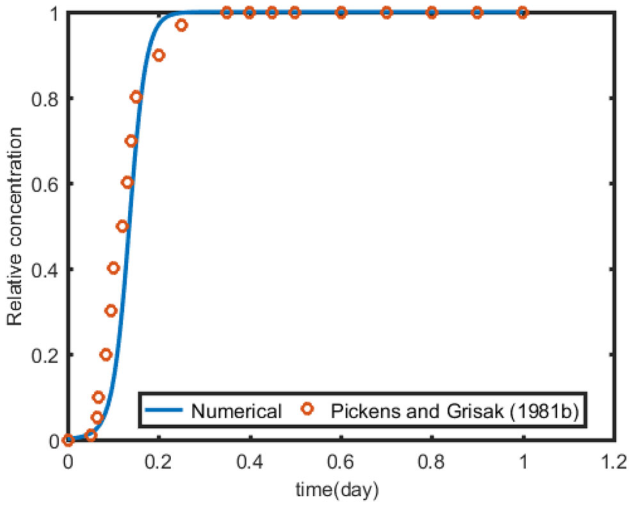

Figure 6. Validation of the numerical solution with analytical solution of the one-dimensional advection-dispersion equation in a homogeneous medium traced by Pickens and Grisak (1981b). Parameters used: dispersivity a = 5 cm; dispersion coefficient =6.7×10^{-6}cm^2/s; total duration of the simulation = 1 day; and domain length = 1m.

Abbreviation

The followings symbols are used in this paper.

D (x)	Depth-dependent dispersion coefficient	L^2T^{-1}
D_0	Molecular diffusion coefficient	L^2T^{-1}
k (x)	Depth-dependent adsorption coefficient	L^3M^{-1}
k_0	Adsorption coefficient in the topsoil	L^3M^{-1}
θ	Soil porosity	–
v_0	Fluid flow velocity	LT^{-1}
R (x)	Depth-dependent retardation factor	–
C	Solute concentration	ML^{-3}
Co	Source concentration	ML^{-3}
x	Observation thickness	L
$\alpha(x)$	Depth-dependent asymptotic dispersivity	
a	Asymptotic dispersivity constant	L
b	Characteristic distance	L
t	Time variable	T
x_0	Transition zone	L
w	Frequency	T^{-1}
λ	Decay rate constant	T^{-1}
L	Length of the finite spatial domain	L
ρ_s	Soil density	ML^{-3}
$t_{1/2}$	Half-life time	T
i, j	Nodes of discretization along (x) and (t)	–
Δx, Δt	Spatial and temporal steps	L, T

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Research article

Numerical solution of the Burgers equation associated with the phenomena of longitudinal dispersion depending on time

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ABSTRACT

In this study, the Burgers equation governing the time-dependent dispersion phenomena is solved numerically using the finite difference scheme and the Runge-Kutta 4 algorithm with appropriate initial and boundary conditions. Two time-dependent dispersion functions have been implemented to analyze the spatio-temporal variation in the domain. For the values of K_L and $K_A < 1.2$ years, a significant retention of the mass of solute is observed when the dispersion function is asymptotic. The results obtained show that the concentration profiles are similar when the values of K_L and $K_A \geq 1.2$ years. These results demonstrate the importance of the nature of the dispersion function on the retention capacity of solutes in the porous medium.

1. Introduction

The fate of properties such as salinity in underground media is of great interest due to increasing concern about the deteriorating environment and human health caused by poor quality groundwater (Ghafari et al., 2020). The transport of dissolved contaminants by heterogeneous hydrogeology is based on expressions of their functional parameters. Several processes acted simultaneously on the chemical constituents transported through the soil. This requires that quantitative descriptions of chemical transport include feasible processes such as the intensity of uptake of contaminants from the subterranean environment. Predicting the concentration of pollutants in the soil matrix is very important to minimize the risk and vulnerability of aquifers (Xie et al., 2019). In addition, the accuracy of the predicted model is crucial to adequately assess and predict the behavior of contaminant transport in the subsoil. Solute transport in groundwater systems is traditionally modeled by the classical non-linear advection-dispersion equation which can add to equilibrium uptake and first order degradation (Ding et al., 2021). The common hypothesis of the dispersion of pollutants in aquifers with constant porosity, regular infiltration flow rate and dispersion coefficient has been approached by many researchers from different angles. Here are some examples. Xue et al. (2020) relied on the new algorithm obtained by the precision of the Crank-Nicolson scheme to solve two-dimensional parabolic equations by alternating the implicit technique of direction. Kumar and Unny (1977) focussed his research on the application of Runge-Kutta methods to solve nonlinear partial differential equations using a specific fluid flow problem. Runge-Kutta of order 4 (RK4), remains up to date a very powerful tool for solving ordinary and partial differential equations. It has the advantage of being simple to program and quite stable for the current functions of physics (Kumar and Unny, 1977; Barletta et al., 2020). Most research has been directed towards improving the precision or flexibility of the classic method from Runge-Kutta methods.

Vázquez-Suñé et al. (2004) considered dispersivity as the most important and difficult parameter to assess in seawater intrusion models, in order to assess the effect of spatial variability of hydraulic conductivity on effective dispersion in seawater intrusion problems. Jaiswal et al. (2011) relied on an analytical solution of the advection-dispersion equation of an input concentration constant along an unstable horizontal flow in a semi-infinite shallow aquifer to determine the level of pollutants in groundwater. Corey et al. (1970), Warrick et al. (1971) have conducted field and experimental studies, and they have suggested that the coefficient of dispersion is not constant but increasing with time.

An unconditionally stable Crank-Nicolson finite difference scheme was used by Ravi et al. (2014) to analyze the constant and longitudinal dispersion profile of contaminants. In his studies, Ravi et al. (2014) did not take into account the time-dependent dispersions coefficients, the decay rate constant and the zero-order production rate coefficient

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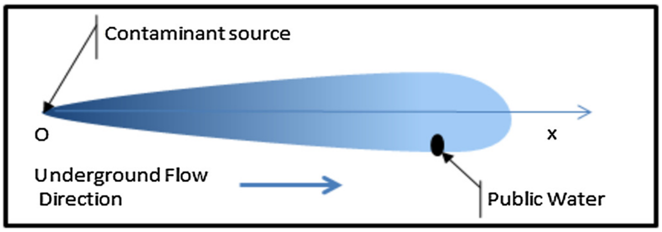

Fig. 1. Infiltration and dispersive system of pollutants in the porous medium.

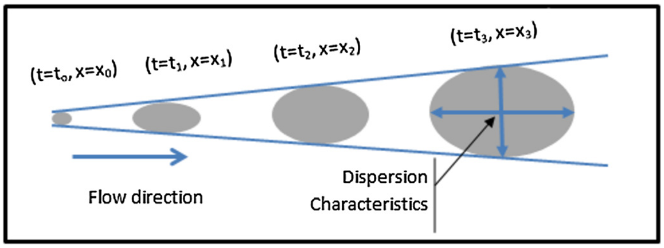

Fig. 2. Geometry of the time-dependent dispersion problem.

of solute in the liquid phase as done by Das et al. (2017), Guleria et al. (2020) with a linear dispersion advection equation model. Our objective is to exploit the more stable fourth-order Runge-Kutta method (RK4) to evaluate the profile of C (X, T) contaminants through a porous medium and to conduct a comparative study between the profiles of the contaminants obtained from an asymptotic and linear dispersion coefficient, and on the other hand, from the initial and boundary conditions used in the work of Das et al. (2017). The discussion will focus on determining the dispersion parameters related to the concentration profiles using the two time-dependent dispersion coefficients.

2. Materials and methods

2.1. Physical model

Water containing pollutants such as sewage eventually seeps into the aquifer which is a reservoir of drinking water. As water passes through the soil, pollutants are mixed, adsorbed, dispersed and diffused by the flowing stream Fig. 1. Several efforts are being made by the scientific community to develop more precise and economical models capable of predicting the transport and concentration of solutes in unsaturated soils. The transport and mixing of contaminants is governed by the advection and dispersion equation of pollutants in the terrestrial aquifer Xie et al. (2019).

2.2. Physical description of the time-dependent dispersion coefficient

Dispersion is a physical phenomenon that occurs when moving away from the injection site, the mass of solute dilutes with time to occupy an increasing volume with a correspondingly decreasing concentration see Fig. 2.

2.3. Mathematical model

Over the past decades, a large number of analytical and numerical solutions have been developed to estimate the fate and transport of various constituents in the underground environment. The application of these solutions is generally limited to non-variable subterranean flow fields and relatively simple initial and boundary conditions nevertheless; these solutions play an important role in contaminant transport studies, providing initial or rough estimates of the distribution of solute concentrations in soils and aquifer systems. The convection-dispersion equation has remained the basis of most analytical and numerical studies of solute transport. The dispersion equation which describes the distribution of the concentration of miscible fluids (i.e. water contaminated or salted with fresh water) in heterogeneous underground media remains one-dimensional in the direction of flow fluids along the x axis (ox) and the other oy and oz components become negligible. The transport equation can be written as equation (1) (Kajal et al., 2014; Singh et al., 2015):

$$\frac{\partial C}{\partial t} + \left(\frac{1-\phi}{\phi}\right)\frac{\partial F}{\partial t} = D_L\frac{\partial^2 C}{\partial x^2} - v_{0x}\frac{\partial C}{\partial x}. \tag{1}$$

Where C is the concentration of the contaminated fluid, F is the concentration in the solid phase, ϕ the porosity of the medium, with D_L the longitudinal dispersion coefficient on the macroscopic scale, and (v_{0x}) the component of the infiltration rate of salt water along the x-axis, and L is the length of dispersion in the direction of flow. Two cases were considered by Lapidus and Amundson (1952) for the solid phase concentration and its derivative, which are equations (2) and (3):

$$F = k_1 C - k_2, \tag{2}$$

$$\frac{\partial F}{\partial t} = k_1 C - k_2 F. \tag{3}$$

Here there is an equilibrium and unbalanced relationship between the concentrations in the two phases. k_1 and k_2 are the constants generally referred to as the order factor for the distribution of pollutants in aquifers. By combining the equations (3) and (2) in (1), we obtain equation (4):

$$R\frac{\partial C}{\partial t} = D_L\frac{\partial^2 C}{\partial x^2} - v_{0x}\frac{\partial C}{\partial x} \tag{4}$$

Where R is the delay factor describing the adsorption of solutes in the porous medium, its expression is equation (5):

$$R = \left(1 + \frac{1-\phi}{\phi}k_1\right). \tag{5}$$

The component of the infiltration rate is related to the dispersal concentration of the pollutant. Ravi et al. (2014) assumes that the rate of infiltration is v_{0x} inversely proportional to the concentration of the pollutant as given in equation (6):

$$v_{0x} = \frac{C(x,t)}{C_0}. \tag{6}$$

This infiltration rate is the cause of the nonlinearity in the advection – dispersion equation. $\frac{1}{C_0}$ represents the proportionality concentration of salt water dispersion. The new parameters of the independent variables introduced to simplify equation (4) are defined as $T = \frac{Rt}{L}$ and $X = \frac{xC_0}{L}$.

Therefore, equation (4) reduces to equation (7):

$$\frac{\partial C}{\partial T} = D_L\frac{\partial^2 C}{\partial X^2} - C\frac{\partial C}{\partial X}. \tag{7}$$

2.4. Description of the time-dependent dispersion model

Field and experimental evidence from studies has been suggested by Corey et al. (1970), Warrick et al. (1971), Sauty (1980), Pickens and Grisak (1981), Sposito et al. (1986) that the dispersion coefficient is not constant but apparently increasing as a function of the displacements in time or equivalently with the distance of displacement of the solute. The apparent increase in the dispersion coefficient has been called the scale effect (Fried and Combarnous, 1971). The scale effect is generally attributed to the heterogeneity of the porous formation, in particular in the heterogeneity of the hydraulic conductivity. Stochastic analyzes have shown that the dispersion depends on the transport time and increases until it reaches an asymptotic value (Gelhar et al., 1979). The theoretical deterministic analysis of Bourgeois (1984) also established that the dispersivity in a stratified aquifer is time dependent. Therefore, there is ample evidence that the dependency scale causes dispersion to vary over time. Therefore, a time-dependent dispersion model can be used to provide a rough description of the transport scale in our study

Table 1. Parameters of the time-dependent dispersion coefficient.

Parameters	Values	Parameters	Values
D_0(L)	5.89 cm^2/min	D_0(A)	4.51 cm^2/min
K$_L$	4500 min	K$_A$	200 min
D_m	0 cm^2/min	D_m	0 cm^2/min

by exploiting the Burger equation. In this study, a linear and asymptotic form of the time-dependent dispersion coefficient is integrated into the nonlinear PDE equation (7) to study the phenomena of longitudinal dispersion of solutes in the underground environment; this has been mentioned in various works (Guleria and Swami, 2018; Guleria et al., 2020). This type of dispersion will make it possible to better represent the results for a transport of solutes in a given porous medium. The time-dependent dispersion coefficient is studied in two forms in this work and equation (7) becomes equation (8):

$$\frac{\partial C}{\partial T} = D_L(T)\frac{\partial^2 C}{\partial X^2} - C\frac{\partial C}{\partial X}. \tag{8}$$

2.5. Time dependent linear dispersion function

The time-dependent linear dispersion increases with time without boundary conditions in the porous medium (Gao et al., 2010; Guleria et al., 2020). The linear formula for the time dependent dispersion expression in equation (8) is given by equation (9) below:

$$D_L(T) = D_0\frac{T}{K_L} + D_m. \tag{9}$$

2.6. Asymptotic dispersion function depend on time

The time-dependent asymptotic distance initially increases with time and eventually approaches an asymptotic value in the porous medium (Guleria et al., 2020). The formula for time-dependent asymptotic dispersion expression in equation (8) is given by equation (10) below:

$$D_L(T) = D_0\frac{T}{K_A + T} + D_m. \tag{10}$$

Where D_0 is the maximum dispersion coefficient for the asymptotic time-dependent and uniform dispersion function for the linear time-dependent dispersion coefficient; D_m is the effective diffusion coefficient of time; K_A is the time-dependent asymptotic coefficient equivalent to the mean distance travelled by the pollutants in the aquifer; K_L is the linear coefficient depending on time. The values of the parameters of the time-dependent dispersion coefficient were determined by a sensitivity analysis of Barry and Garrison (1989). The same values of the parameters of the linear and asymptotic time-dependent dispersion coefficient exploited in the work of Guleria et al. (2020) which are also exploited in this work, are presented in the Table 1.

Fig. 3 illustrates the analysis of the asymptotic limit of the time-dependent dispersion coefficient given in relation 10, which remains important and more practical in porous media. The values of K$_A$ depend on the extent of the pre-asymptotic zone. K$_A$ equal to zero indicating constant dispersion. The smaller the value of K$_A$, the more the dispersion approaches the asymptotic value. The values of K$_A$ other than zero corresponding to the times for which the dispersion reaches half of its asymptotic value.

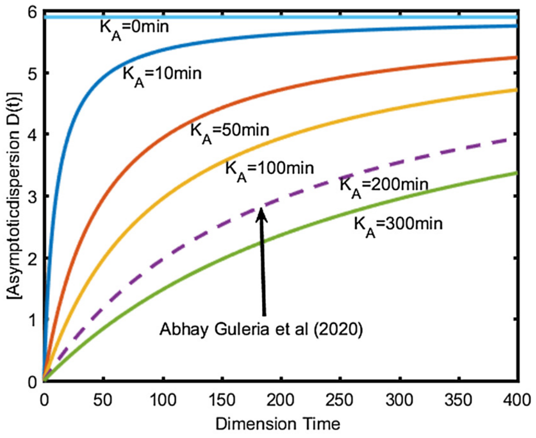

Fig. 3. Asymptotic dispersion coefficient for various K$_A$ using data from Table 1.

2.7. Initial and boundary conditions

From the source of the pollutants, the concentration disperses more in the porous medium in the direction of flow with a front at the arrival of the boundary see Fig. 4. At the initial moment it is assumed that the aquifer is contaminated, a certain initial background concentration exists in the aquifer and it is represented by a linear combination of an initial concentration and the term of zero order production with rapid infiltration given by equation (11):

$$C(X,0) = C_i + \frac{\gamma X}{v_{0x}}, \quad X > 0,\ T = 0 \tag{11}$$

Where C_i is the initial background concentration, v_{0x} is flow velocity, and γ is the zero order production rate coefficient for liquid phase solute production. A contaminant in radioactive waste decaying exponentially with time is imposed upon entering the aquifer as a linear combination of a source concentration with an initial background concentration at the origin, to describe the transport of solutes in a natural or artificial system as expressed by equation (12) (Das et al., 2017; Singh et al., 2021):

$$C(0,T) = C_i + C_0\exp(-\lambda T), \quad T > 0,\ X = 0, \tag{12}$$

λ is the decay rate constant and v_{0x} is the flow velocity of fluids in the porous medium.

At the other end of the aquifer, solute transport may not be affected and therefore an exit boundary condition is prescribed as a non-flow boundary condition (Das et al., 2017). The mathematical expression of these phenomena is expressed by equation (13) as:

$$\frac{\partial C}{\partial X} = 0, \quad X \to \infty. \tag{13}$$

2.8. Numerical solution of the mathematical model

The one-dimensional solute transport equation is a parabolic-type partial differential equation in which the finite difference technique is commonly used to obtain the numerical solution (Togue-kamga et al., 2012). An explicit finite difference technique is usually used, and ultimately results in restrictive stability criteria Das et al. (2017).

2.9. Fourth-order Runge-Kutta (RK4) method

The numerical technique is used to solve the equation (8) expressed as equation (14) (Togue et al., 2019; Kumar and Unny, 1977):

$$\frac{\partial C}{\partial T} = f(T, C(T)). \tag{14}$$

The semidiscrete equation (14) is solved using the RK4 scheme according to the algorithm given by equation (15):

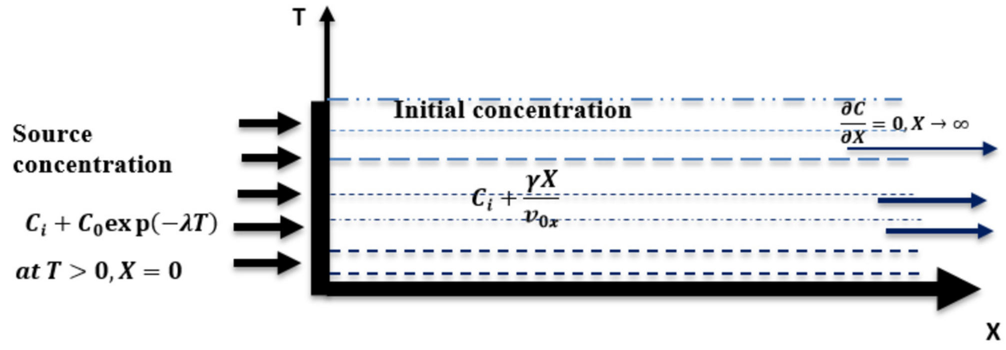

Fig. 4. Geometry of the problem.

$$\begin{cases} K_1 = \Delta T\, f(T, C(T)) & \text{(a)} \\ K_2 = \Delta T\, f(T + \frac{1}{2}\Delta T, C(T) + \frac{1}{2}K_1) & \text{(b)} \\ K_3 = \Delta T\, f(T + \frac{1}{2}\Delta T, C(T) + \frac{1}{2}K_2) & \text{(c)} \;. \\ K_4 = \Delta T\, f(T + \Delta T, C(T) + K_3) & \text{(d)} \\ C(T, \Delta T) = C(T) + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) & \text{(e)} \end{cases} \tag{15}$$

With (ΔT) the time step, C(T) the value of the pollutant concentration at time t and C(T + ΔT) the value of the pollutant concentration at time (T + ΔT).

The derivatives of the equation (8) are approximated by the truncated expansion of the numerical finite difference approximation scheme to determine the first and second order spatial derivatives are obtained from equations (16) and (17) (Natarajan et al., 2020):

$$\frac{\partial C}{\partial X} = \frac{C_i^j - C_{i-1}^j}{\Delta X}, \tag{16}$$

$$\frac{\partial^2 C}{\partial X^2} = \frac{C_i^{j+1} - 2C_i^j + C_{i-1}^j}{\Delta X^2}. \tag{17}$$

The first order temporal discretization is given by equation (18) written as:

$$\frac{\partial C}{\partial T} = \frac{C_i^{j+1} - C_i^j}{\Delta T}. \tag{18}$$

The indices (i) and (j) indicate the nodes of discretization along (X) and (T) respectively. ΔX is the spatial step. Thus, equation (8) can be written in a discrete form such as equation (19):

$$\frac{\partial C_i^j}{\partial T} = f(X, T, C_{i+1}^j, C_i^j, C_{i-1}^j). \tag{19}$$

Where the function $f\left(X, T, C_{i+1}^j, C_i^j, C_{i-1}^j\right)$ in equation (19) is expressed as equation (20):

$$f(X, T, C_{i+1}^j, C_i^j, C_{i-1}^j) = D(j)\left(\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta X^2}\right) - C_i^j\left(\frac{C_i^j - C_{i-1}^j}{\Delta X}\right), \tag{20}$$

$X = i\Delta X$, $T = j\Delta T$, with (i = 0,1,2,...,Nx) and (j = 0,1,2, ...,Nt).

The discretization of boundary and initial conditions is necessary to apply this method. The discrete equation of the initial condition and boundary conditions associated with equation (11), (12) and (13) is expressed as equation (21):

$$\begin{cases} C_i^0 = C_i + \frac{\gamma X_i}{v_{0x}}, & i > 0,\ j = 0, \quad \text{(a)} \\ C_i^0 = C_i + C_0 \exp(-\lambda T_j), & j > 0,\ i = 0 \quad \text{(b)} \\ \frac{\partial C_{N_x}^j}{\partial x} = 0, & j > 0. \quad \text{(c)} \end{cases} \tag{21}$$

2.10. *Stability condition*

Equation (8) can be written in the discrete form as equation (22) below:

$$C_i^{j+1} = (1 - 2\alpha)C_i^j + \alpha C_{i+1}^j + \alpha C_{i-1}^j + \beta C_i^j (C_i^j - C_{i-1}^j). \tag{22}$$

The coefficients α and β defined in equation (22) are expressed in equation (23) and (24):

$$\alpha = \frac{D_j \Delta T}{\Delta X^2} \tag{23}$$

$$\beta = \frac{\Delta T}{\Delta X} \tag{24}$$

This implies that the condition of stability of equation (22) is expressed as equation (25):

$$\begin{cases} 0 \le 1 - 2 \propto \le 1 & \text{(a)} \\ 0 \le \propto \le 1 & \text{(b)} \\ 0 \le \beta \le 1 & \text{(c)} \end{cases} \tag{25}$$

For the conditions of stability equation (25), the coefficients α and β defined in equation (22) must be positive as expressed in equations (26) and (27), thus

$$\alpha = \frac{D_j \Delta T}{\Delta X^2} \succ 0 \tag{26}$$

$$\beta = \frac{\Delta T}{\Delta X} \succ 0 \tag{27}$$

From equation (25), we obtain the stability condition which is expressed as equation (28):

$$0 \le \Delta T \le \frac{\Delta X^2}{2D_j}. \tag{28}$$

These inequalities fix a strict maximum limit to the size of the time step and represent a serious limitation for the centered finite difference diagram.

3. Results and discussion

3.1. *The spatial and temporal variation in the concentration*

We analyzed the numerical solutions using the following model parameters: $C_i = 0.01$, $D_0 = 0.1$ km^2/year $\lambda = 0.001$ $v_{0x} = 0.01$ km/year, $\gamma = 0.0007$ (Das et al., 2017; Guleria et al., 2020; Natarajan, 2016). Figs. 5a and 5b illustrate the spatial and temporal variation in the concentration of the contaminant for different values of K_A and K_L $(0.2, 0.7, 1.2, 1.7$ years).

Fig. 5a illustrates the spatial distribution of the concentration of pollutants by considering the different values of K_L and K_A. The spatial concentration profiles decrease exponentially in the aquifer for the values of K_L and K_A (0.2 years, 0.7 years, and 1.2 years). This profile

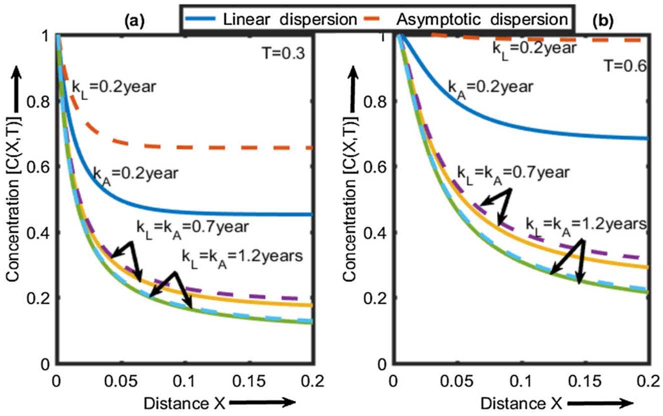

Fig. 5. Spatial representation of the concentration C (X, T) for de T = 0.3 (a) and T = 0.6 (b) according to the different values of K_L and K_A.

decreases rapidly when the dispersion function is asymptotic, reflecting greater retention of the mass of solute in the medium. These results are similar to those obtained by Guleria et al. (2020). These authors have studied time moments (concentration per unit time) to interpret the behavior of the solute plume in porous media such as porous media laminated hydraulically with a dispersion as a function of time. The different concentrations all decrease together from the entry of the aquifer independently of the dispersion coefficient, to reach horizontal asymptotes at the different positions X = 0.029, 0.054, 0.058 respectively for three values of K_A (0.2 years, 0.7 years, 1.2 years). The percentage of residual concentration associated with these positions is 0.76; 0.30; 0.24. On the other hand, the different horizontal asymptotes are rather obtained at the different positions X = 0.04, 0.055, 0.058 respectively for the values of K_L (K_L = 0.2 years, 0.7 years, 1.2 years). The associated residual concentration percentage is 0.55; 0.28; 0.24. These positions grow with the increase of K_L and K_A. The percentage of residual solute concentration remains low when the dispersion function is asymptotic. These results confirm that the increase in K_A assigned to asymptotic time-dependent dispersion coefficients significantly reduces the mass of solute in the subterranean medium compared to K_L associate with linear dispersion coefficients. The concentration profiles in the porous medium get closer when the characteristic K_L and K_A of the medium increase. For the values of K_L and $K_A < 1.2$ years, a significant retention of the mass of solute is observed when the dispersion function is asymptotic. A similarity of the concentration profiles is observed for the value of K_L and $K_A \geq 1.2$ years. This similarity of the concentration profile is due to the temporal variation of the effective dispersion coefficient without upper limit in the underground medium (Guleria et al., 2020).

Fig. 5b shows that the retention of the mass of solute gradually decreases compared to that observed in Fig. 5a. Likewise, for the values of K_L and $K_A < 1.2$ years, a significant retention of the mass of solute is observed when the dispersion function is asymptotic. Also, an analogy of the concentration profiles is observed for the value of K_L and $K_A \geq 1.2$ years.

4. Conclusion

In this study, the Burgers equation associated with a linear and asymptotic time-dependent dispersion function was numerically simulated to determine the spatiotemporal variation in concentrations. Analysis of the results shows that the concentration profiles decrease rapidly when the dispersion function is asymptotic, reflecting greater retention of the mass of solute in the medium. Values of K_L and K_A for which the concentration profiles are similar were determined. These results demonstrate the importance of the nature of the dispersion function on the retention capacity of solutes in the porous medium.

Declarations

Author contribution statement

Calvia Yonti Madie: Performed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Fulbert Kamga Togue, Paul Woafo: Conceived and designed the experiments; Analyzed and interpreted the data.

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Data availability statement

Data will be made available on request.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

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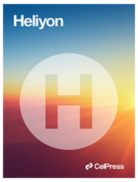

Research article

Dispersion of pollutants in a porous medium with finite thickness and variable dispersion coefficients

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ABSTRACT

Groundwater is subject to the intrusion of pollutants of various types. These pollutants can have natural or anthropogenic sources. Their consumption can therefore affect human health, but also affects the development of vegetation. The objective of this article is to analyze the effect of the dispersion coefficient parameters on the spatio-temporal distribution of pollutants in a saturated porous medium with a finite thickness. This layer is subjected to two types of conditions at the outlet of the aquifer where the dispersion coefficient is a function of depth. The partial differential equations were solved using an implicit finite difference technique. The results of the analysis suggest that the behavior of the concentration profile was influenced by the different output boundary conditions. On the other hand, the parameter, b of the dispersion coefficient depending on the distance has a significant impact on the movement of the solute in a saturated porous medium compared to the parameter, a. In other words, it has more effect on the dispersion of pollutants in aquifers. This study highlights the need to bring insight on the transports parameters while modeling the transport of solute in a porous media.

1. Introduction

The problem of the dispersion of solutes during the movement of fluids was at the center of interest at the beginning of this century, but it was not until 1905 that the general theme of hydrodynamic dispersion or miscible displacement became one of Ravi's most systematic studies (2014); Patel et al. (2014). The mathematical statement of the solute transport equation, also called the advection-dispersion equation, has been accepted as a model to describe the migration and position of solutes in groundwater Patel et al. (2014); Xie et al. (2019). For a particular case, the equation includes evolutionary and dispersive transport processes. Advection-dispersion equation models are used to describe the movement of solutes in porous media and also allow for the rapid location of water potability sites in these media. Analytical and numerical solutions of these, generated by initial boundary conditions, remain an essential tool for environmentalists, hydrologists, civil engineers, and mathematical modelers to examine the process of remediation and management of a contaminant in a hydro-environment and to validate their experimental work (Pickens and Grisak, 1981).

The use of the coefficient of dispersion of pollutants in groundwater has been discussed by many researchers from different angles. Here are some examples. Depth-dependent dispersion was experimentally justified by Pickens and Grisak, 1981, as he reorganized several transport assays from fields and laboratories to predict the transport of contaminants in heterogeneous porous media. The accuracy and capability of the scale-dependent dispersion model in a heterogeneous medium was simulated by Pickens and Grisak, 1981 across heterogeneous soil using the values of the asymptotic dispersivity, $a = 20$ m and the characteristic half of its length, $b = 50$ m. Hamza (2003) relies on a particular solution derived from various diffusion functions and mass injection scenarios which includes the linear, asymptotic and exponential variation of the diffusion functions to evaluate the migration of the solute with a time-dispersion dependent coefficient with the three scenarios.

Djordjevich and Savović (2013) used the implicit finite difference method to solve the advection-dispersion equation in their work. This method is unconditionally stable and yet it does not result in higher computational efficiency because extremely large matrices have to be manipulated at each computational step. The finite difference method is also easier to program in addition to being more computationally efficient Savović and Djordjevich (2013).

Other researchers have used the term speed-dependent dispersion to assess numerically using a specific technique based on an adaptive

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scheme. They also showed that the numerical integration and the nonlinear dependence of the dispersion with respect to velocity make the semi-analytical solution impractical Fahs et al. (2016). Abgaze and Sharmar (2015) present in the first part of their study, constant, linear and asymptotic dispersion coefficients as a function of distance to describe the scaling effect and to simulate the experimental fracture curves observed in a column and simulate experiments with long, thin soils. A comparative study was carried out between distance-dependent dispersion and constant dispersion, simulating experimental data on the transport of solutes in the soil's column with a constant mass transfer coefficient. Yan et al. (2015) proposed an empirical correlation describing the interaction of asymptotic behaviors of longitudinal and transverse dispersion of the solute for flow through packets of random particles. Dagan (1984) used a similar approximation by satisfying a diffusion equation with time-dependent apparent dispersion coefficients to determine the expected value of the concentration. Lee et al. (2018) used the meaning of local equilibrium when examining with local equilibrium to model longitudinal dispersion in groundwater. Silliman and Simpson (1987) performed laboratory work using various tests to assess changes in dispersivity caused by the presence of heterogeneities. Molz et al. (1983) relied on the definition of a scale-dependent macro dispersion coefficient to study a unidirectional flow in a stratified aquifer, then obtained for the macro-dispersivity the different components within a limited time.

A semi-analytical solution of the transport model with an asymptotic dispersion depending on the distance and on the asymptotic dispersivity parameters (a), and on the half-length characterizing the mean stroke (b), was developed by Sharma and Abgaze (2015) taking into account a condition of zero pollutant concentration at the outlet of the domain and parameters of constant asymptotic dispersivity in a homogeneous porous medium. This author neglected certain boundary conditions that may occur at the aquifer boundary due to natural phenomena, as mentioned in the works of Al-Niami and Rushton, (1976); Yadav et al. (2012) and the variability of the asymptotic dispersivity parameters in a heterogeneous porous medium.

In our recent study Madie et al. (2022a), the advection dispersion equation was solved numerically to evaluate the concentration profile of salinity in aquifers for a distance-dependent dispersion coefficient problem. A distance-dependent adsorption coefficient and a constant asymptotic dispersion parameters a and b were also considered. Three initials concentration injection condition were introduced at the inlet of the aquifer: (a) constants, (b) variables exponentially with time and (c) sinusoidally with time.

This article proposes a numerical solution of the transport model with an asymptotic dispersion dependent on the distance with the parameters of asymptotic dispersivity (a), and the half-length characterizing the mean stroke (b) developed by Sharma and Abgaze (2015), by taking two conditions at the outlet of the domain and a variable asymptotic dispersion parameters a and b in a heterogeneous porous medium.

Our objective is to examine the impact of the asymptotic dispersion parameters on the spatio-temporal variation of pollutant concentration in the underground environment.

2. Materials and methods

2.1. Description of the physical model

Figure 1 illustrates the physical model of the problem. In this model, dispersion coefficient varies with respect to the depth, x, one-dimensional and the Darcy velocity is constant. The boundary conditions are defined at the boundaries of the matrix.

2.2. Mathematical description

The heterogeneity of most geological materials is caused by certain natural deformations, such as fractures, and lenses of high or low permeability which are at the origin of the variation of the hydraulic properties and the spatial or temporal increase of the dispersivity in the porous medium (Kangle et al., 1996; Madie et al., 2022b). Most geological materials are extremely inhomogeneous due to the presence of irregular stratifications, cracks and fractures and lenses of high or low permeability. These non-homogeneities cause the hydraulic properties to vary in space, leading to fluctuations in the speed of the fluid, and eventually give rise to a dispersivity which increases with distance or time. Field and experimental evidence from studies has been suggested by Pickens and Grisak, 1981 that the dispersion coefficient is not constant but apparently increasing with time displacement and distant traveled by the solute. The phenomenon of dispersion is a phenomenon which moves away from the place of injection, the mass of solute is diluted during its displacement along the direction of flow x to occupy an increasing volume with a relatively decreasing concentration. The latter suggests that in a heterogeneous medium the pollutants transport equation taking into account a constant dispersion parameter become unsuitable, for this reason the distance-dependent dispersion coefficient is applied in the advection-dispersion equation below Madie et al. (2022a).

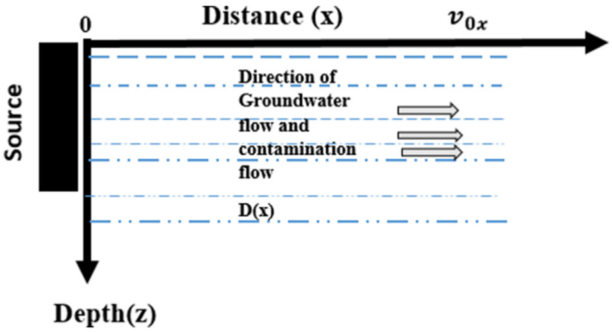

Figure 1. Physical model of the system.

The transport equation, defining the variation in concentration as a function of time and space of a dissolved substance transferred into a heterogeneous saturated porous medium, is written as the linear Eq. (1) form Sharma (2015); Yadav (2018):

$$R\frac{\partial c}{\partial t}=D(x)\frac{\partial^2 c}{\partial x^2}-v_{0x}\frac{\partial c}{\partial x} \tag{1}$$

This equation involves two major terms influencing the transfer potential of the solute through a saturated porous medium. c is the concentration of the pollutants, R a delay factor generated by the absorption of the pollutant, t time and x distance traveled by the fluid in the porous medium. Convection or fluid flow velocity (v_{0x}) describes the transport of a solute by the movement of a fluid moving through a porous medium Gao et al. (2010). This water flow in a saturated porous medium (absence of gas in the pores) is defined by the following relation: $v_{0x} = q/\theta$ or $q = ki$ (Darcy flow) and θ: the effective porosity of the medium; k: the permeability of the aquifer, i: the hydraulic gradient of the aquifer (Figure 1).

2.3. Physical description of the distance-dependent asymptotic dispersion coefficient parameter

The variation of many subsurface parameters caused by natural disaster makes it difficult to use the dispersion-advection equation with a single parameter to predict the concentration of contaminants at different distances in a porous medium. The asymptotic dispersivity is a physical quantity considered to account for the heterogeneity of porous media. Asymptotic dispersivity, which depends on the distance travelled by the fluids, is used to define the notion of a distance-dependent dispersion model for solute transport in heterogeneous porous media (Kangle et al., 1996; Madie et al., 2022a). The hydrodynamic dispersion coefficient D (x) which is a function of the distance in the homogeneous porous medium in the absence of any molecular diffusion due to very fine tortuosity is written as Eq. (2) below:

$$D(x) = D_0 + \alpha(x)v_{0x} \tag{2}$$

where α (x) is the dispersivity and $D_0 = [D_e\tau]$ is the molecular diffusion caused by molecular motion and particle collisions; with $\tau \leq 1$: tortuosity of the porous medium, D_e is the effective dispersion. Asymptotic dispersivity is responsible for the heterogeneity of porous media and it initially increases with the distance traveled and eventually approaches an asymptotic value, Yan et al. (2015). Since the asymptotic dispersion coefficient depends on the distance, such a relation can be expressed Eq. (3) below:

$$D(x) = D_0 + a\left(1 - \frac{b}{x+b}\right)v_{0x} \tag{3}$$

where a is the value of the asymptotic dispersivity and b is a characteristic distance which determines the distance of displacement for the dispersivity to reach half of the asymptotic value. Dispersivity is the ratio of the asymptotic dispersion coefficient to the pore velocity of water. The values of b depend on the extent of the pre-asymptotic zone. For a smaller value of b, the dispersivity will approach the asymptotic value more quickly. The accuracy and capability of the scale-dependent dispersion model in a heterogeneous medium was simulated by Pickens and Grisak (1981) across heterogeneous soil using the experimental values of the asymptotic dispersivity, a = 20 m and the characteristic half of its length, b = 50 m and no molecular diffusion.

2.4. Initial and boundary conditions

We consider a horizontal unidirectional flow of water through an aquifer of finite length L, with an initial concentration c_0 at the inlet of the aquifer, the movement is rather in the direction of the flow x. The concentration water infiltrates into the soil matrix, then, influenced by the parameters of the soil, and becomes a source of drinking water at zero concentration at the arrival of the boundary for L infinite Madie et al. (2022a). The problem can be defined mathematically by Eq. (1) with the following initial and boundary conditions given by Eq. (4):

$$\begin{cases} c(x,0) = 0; \textit{for } 0 < x < L \\ c(0,\ t) = c_0 \textit{ for all } t, \\ c(L,t) = 0 \textit{ for } t > 0 \end{cases} \tag{4}$$

The boundary condition of Eq. (4) assumes that the concentration at (x = L) is held to zero at all times as shown by the work of (Sauty (1980); J. W. Biggar and Nielsen (1971), this may not always happen in practice. An alternative condition which allows a certain dispersion to occur at the boundary is given by Eq. (5):

$$\begin{cases} c(x,0) = 0; \textit{for } 0 < x < L \\ c(0,\ t) = c_0 \textit{ for all } t, \\ \dfrac{\partial c}{\partial x}(L,t) = \dfrac{v_{0x}}{2D(x)}c(L,t) \textit{for } t \geq 0 \end{cases} \tag{5}$$

The boundary condition of Eq. (5) assumes that the amount of pollutants crossing the boundary (x = L) is proportional to the flow producing at the boundary because the accumulation time has not yet arrived, hence the accumulation term of Eq. (1) canceled out ($\frac{\partial c}{\partial t} = 0$) to give rise to this flow. This phenomenon of proportionality at the boundary occurs in practice when poor quality water is prevented from spreading by a flow of fresh water. In practice, the flow is reduced due to natural causes or due to increased exploitation of good quality water and the risk of poor quality water spreading is very high Al-Niami and Rushton, (1976), Yadav et al. (2012).

2.5. Numerical solution of the mathematical model

Finite difference methods are generally used to solve fluid flow equations in porous media. The difference methods allow the calculation of the average load per mesh and provide the exact mass balance at each element. The discretization of the fluid flow equation by finite differences is very obvious and simple to implement, but applicable on rectangular or cubic meshes Wang and Anderson (1982). The derivatives of the fluid flow Eq. (1) are approximated by the finite difference numerical scheme to determine the first and second order spatial derivatives, which are defined from Eqs. (6) and (7) (Natarajan et al., 2020; Madie et al., 2022b):

$$\frac{\partial c}{\partial x} = \frac{c_i^j - c_{i-1}^j}{\Delta x} \tag{6}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{\Delta x^2} \tag{7}$$

The first order temporal discretization is given by Eq. (8) written as:

$$\frac{\partial c}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t} \tag{8}$$

The indices (i) and (j) indicate the nodes of discretization along (x) and (t) respectively. Δx and Δt are respectively the spatial and temporal steps. Thus, Eq. (1) can be written in the discrete form such as Eqs. (9) and (10):

$$c_i^{j+1} - c_i^j = \frac{D_i\Delta t}{R\Delta x^2}\left(c_{i+1}^j - 2c_i^j + c_{i-1}^j\right) - \frac{v_{0x\Delta t}}{R\Delta x}\left(c_i^j - c_{i-1}^j\right), \tag{9}$$

$$c_i^{j+1} = (1 - 2\propto - \beta)c_i^j + \propto c_{i+1}^j + (\propto + \beta)c_{i-1}^j, \tag{10}$$

where $\propto = \frac{D_i\Delta t}{R\Delta x^2}$ and $\beta = \frac{v_{0x\Delta t}}{R\Delta x}$

The discretization of boundary and initial conditions is necessary to apply this method. The discrete version of the initial condition and boundary conditions given successively by Eqs. (4) and (5) is expressed as Eqs. (11) and (12):

$$\begin{cases} c_i^0 = 0,\ \textit{if } 0 \leq i \leq Nx \\ c_0^j = c_0,\ \textit{if } j \geq 0, \\ c_{Nx}^j = 0,\ \textit{if } j > 0 \end{cases} \tag{11}$$

$$\begin{cases} c_i^0 = 0,\ \textit{if } 0 < i < Nx \\ c_0^j = c_0,\ \textit{if } j \geq 0, \\ \dfrac{\partial c_{Nx}^j}{\partial x} = \dfrac{v_{0x}}{2D_i}c_{Nx}^j\ , \textit{if } j \geq 0 \end{cases} \tag{12}$$

These two relationships express a column without contamination at the initial moment where c_o is the concentration of pollutants at the entrance to the aquifer.

2.6. Stability conditions

An approach similar to that used by Natarajan et al., 2020 where the spatial and temporal steps tend to zero, which also leads the error to tend to zero is used to obtained stability conditions. This leads to imposing certain conditions on the finite difference scheme of the discrete Eq. (10) which are given by the following Eq. (13):

$$\begin{cases} 0 \leq 1 - 2\propto - \beta \leq 1 \\ 0 \leq \propto \leq 1, \\ 0 \leq \propto + \beta \leq 1 \end{cases} \tag{13}$$

The new solution is a convex combination of the solution at new time step (j + 1) at a spatial node i is an average of the solutions at the previous

Table 1. Parameter values used to simulate concentration profile.

Parameters	Symbols	Values
Asymptotic dispersivity value	a	20 m
Characteristic distance	b	50 m
Flow velocity	v	0,8 m/d
Retardation factor	R	2.5

time step at the nodes i − 1, i and i + 1. The new solution linked continuously to the initial value of c_i^0. This implies

$$\begin{cases} \beta \leq 1 - 2\propto \leq 1 + \beta \\ 0 \leq \propto \leq 1, \\ -\propto \leq \beta \leq 1 - \propto \end{cases} \tag{14}$$

By simplifying Eq. 14a and 14c, we have $-\propto \leq \beta \leq 1 - 2\propto$

Thus, the stability conditions are $0 \leq \propto \leq 1$ and $-\propto \leq \beta \leq 1 - 2\propto$.

In this work $0 \leq \frac{D_i \Delta t}{R \Delta x^2} \leq 1$ and $-\frac{D_i \Delta t}{R \Delta x^2} \leq \frac{v_{0x\Delta t}}{R \Delta x} \leq 1 - 2\frac{D_i \Delta t}{R \Delta x^2}$. The data in Table 1 were taken from the work of Al-Niami and Rushton (1977); Pickens and Grisak (1981).

3. Results and discussion

3.1. Validation of the model

An analytical solution provided which constant coefficient by Ogata and Banks (1948) is used as shown in Figure 2 to justify the correct implementation of the model. It is observed from Figure 2 that there exists a close agreement between the numerical solution and the analytical solution. Therefore, our model can be used to predict the concentration distribution curves as a function of the thickness of the aquifer with different entry and exit boundary conditions.

3.2. Variation of pollutants concentrations in the system

In this section the discrete Eq. (10) obtained by the finite difference method associated with the initial and boundary conditions of the discrete Eqs. (11) and (12) is solve numerically to obtain the results below.

The numerical solutions of the advection dispersion Eq. (1) is evaluated as a function of aquifer length, time, dispersion coefficient varying as a function of distance traveled and the rate of flow of fluids in the aquifer. For this purpose, the model parameters used are presented in Table 1, were selected in previous studies Guangyao Gao., (2010); Kangle et al. (1996); Wang et al. (2020); Natarajan et al., 2020; N. Natarajan (2015); Al-Niami and Rushton (1976).

The first condition represents the boundary condition presented in Eq. (4) and the second condition is the boundary condition presented in Eq. (5).

Four points were selected in the aquifer (L/4, L/2, 3L/4, 0.9L) to assess the behavior of the dispersion of pollutants in the system. Figures 3 and 4 show the relationship between the evolution of the concentration of pollutants at different points and the dispersion coefficients parameters a and b using the initial and boundary conditions given respectively by Eqs. 4 and 5. Higher values of pollutant concentrations are obtained near the source (x = L/4) while low values were found near the outlet of the system (x = 0.9 L). These results show that the dispersion of pollutants increases with the distance of transport. Figures 3 and 4 inform us about the points that were exploited by Sharma and Abgaze. (2015) from the entrance to the exit of the aquifer, because in their work they considered the value a = 0.8273 m and b = 1.4821 m. Chen et al. (2008) as from them, they rather fix the value a = 0.284 m and b = 10 m. In the light of Figures 3 and 4, it appears that the data for the values of a and b used in these cited work are well located in a specific zone of the aquifer according to the selected points. The results also suggest that the parameter b has an important effect on the dispersion of pollutants (Figure 3B) rather than on the asymptotic dispersivity a (Figure 3A).

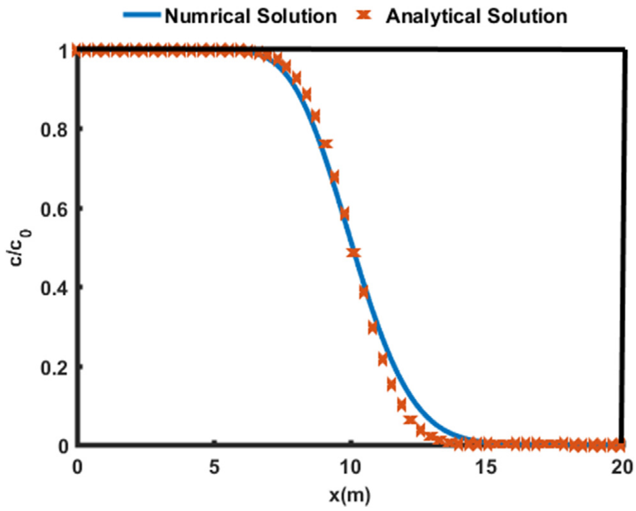

Figure 2. Validation of the numerical solution with analytical solution of the one-dimensional advection-dispersion equation in a homogeneous medium provided by Ogata and Banks (1948). Parameters used: speed = 1 m/d; dispersion coefficient = 0.1 m^2/d; delay factor = 1; total duration of the simulation = 10 days; and domain length = 100 m.

The concentrations are higher in Figure 4 due to the initial and boundary conditions (Eq. 8). For proper environmental modeling of solute transport in porous media, experimental studies should be performed to find the values of parameters a and b rather than fixing them as is done in the literature Guangyao Gao., (2010); Kangle et al. (1996). It is also possible to find the range of these parameters which could improve the performance of the system (Figure 5).

Figures 5 and 6 show the evolution of pollutant concentrations as a function of the various constants of dispersion coefficients a and b near the outlet of the aquifer (0.9 L) for the two cases, where the constraints of the pollutants are zero (Figure 5) and not zero (Figure 6). These two Figures should allow us to select the exact values of a and b.

Figures 5(A) and 6(A) shows the spatial variation of the concentration of pollutants in the porous medium for different values of the dispersivity a (a = 4 m, 8 m, 12 m, 16 m, 20 m) of the dispersion function as a function of depth. Figures 5(A) and 6(A) shows that the mass of solute retained in the medium increases with the value of the dispersivity. The concentration profiles follow an exponential decrease in the aquifer independently of the value of the dispersivity a. This result is similar to those of Kangle et al. (1996). These authors analytically solved the one-dimensional dispersion advection equation to predict solute transport in heterogeneous porous media with scale-dependent dispersion. It appears that the mass of solute retained in the porous medium increases with the value of dispersivity a. It is also observed that the slope of the concentration profile becomes closer and closer with an increase in a. This is due to the asymptotic variation of the dispersion coefficient which approaches more and more its asymptotic value in the porous medium.

It was noted in Figure 5(B) that, for b equal to 5 m and for all the values of for a ∈R + in the aquifer, we observe high values of concentrations with a range between 14 and 15% of the initial concentration. It was also noted in Figure 5(B) that, for b equal to 40 m and for all the values of a ∈R + we observe the lowest values of concentrations with a range between 2 and 3% of the initial concentration. From the analysis of the dispersion constants a and b for the stresses of zero concentrations at the outlet of the aquifer, it emerges that the appropriate values of b are equal to or greater than 40 m for all values of for a ∈R +. High concentration values are obtained for b less than 5 m.

Figure 6(B) shows that, for b equal to 5 m, the same trend is observed as in Figure 5(B) for non-zero concentrations at the outlet of the aquifer. However, for b equal to 40 m and for all the values of a ∈R + we observe the lowest values of concentrations with a range between 1 and 2% of the

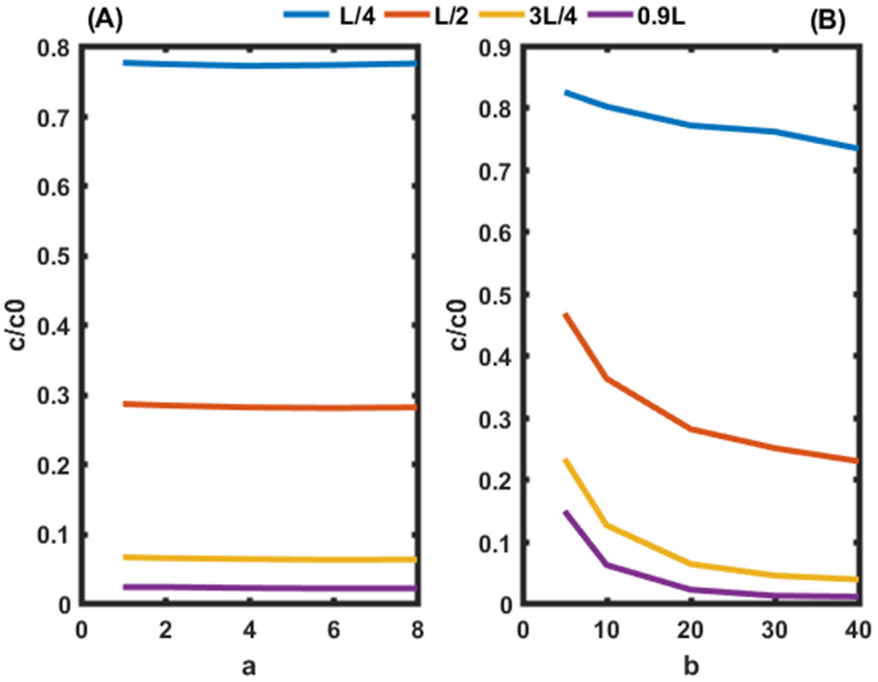

Figure 3. Variation of pollutants concentrations in the system as function of *a* and *b*. In (A) initial and boundary conditions given by the first condition (t = 50 day, R = 2.5, v = 0.8 m/d,a = 8 m). In (B) initial and boundary conditions given by Eq. (7) (t = 50 day, R = 2.5, v = 0.8 m/d, b = 40 m^{-1}).

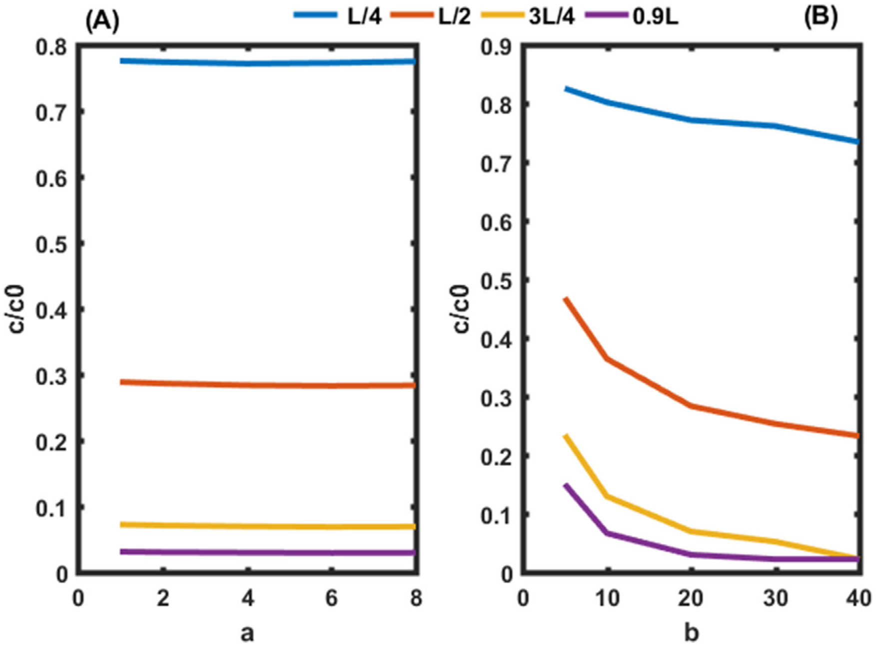

Figure 4. Variation of pollutant concentrations in the system as a function of a and b. In (A) initial and boundary conditions given by the second condition (t = 50 day, R = 2.5, v = 0.8 m/d,a = 8 m). In (B) initial and boundary conditions given by Eq. (8) (t = 50 day, R = 2.5, v = 0.8 m/d, b = 40 m).

initial concentration rather than 2 and 3% as observed on Figure 5(B). These values of b found are used at different points of the aquifer in this work to analyze the effect of the dispersion coefficient as a function of distance and time on the transport of contaminants in porous media (Figure 7).

Figures 7(A) and 7(B) successively illustrate the spatial distribution of the concentration of pollutants with chosen constants dispersion coefficients b = 5 m and b = 40 m. An interesting observation from the graphs above is that the concentration profiles for the two values of b above follow an exponential decay pattern in the aquifer for any value of a (a = 4 m, 6 m, 8 m). These results are similar to those obtained by Kangle et al. (1996). These authors have developed a general analytical solution for one-dimensional solute transport in heterogeneous porous media with scale-dependent dispersion. The results obtained in Figures 7(A) and 7(B) show that by allowing 10% initial concentration (10% of C_0) as a guide value in a porous medium, the suitable points of installation of drinking water points are in the order of x/L = 0.65; 0.53; 0.45 respectively for a = 4 m, 6 m, 8 m and b = 5 m. On the other hand,

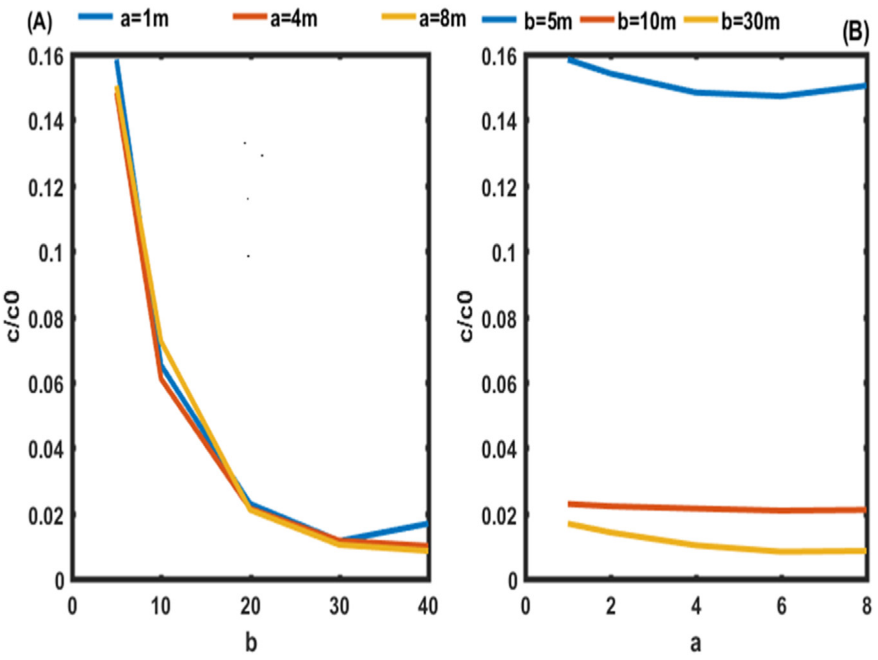

Figure 5. Behavior of pollutants on leaving the aquifer (0.9L) for the first condition. In (A) the behavior of pollutants is given in function of b. In (B) the behavior of pollutants is given in function of a.

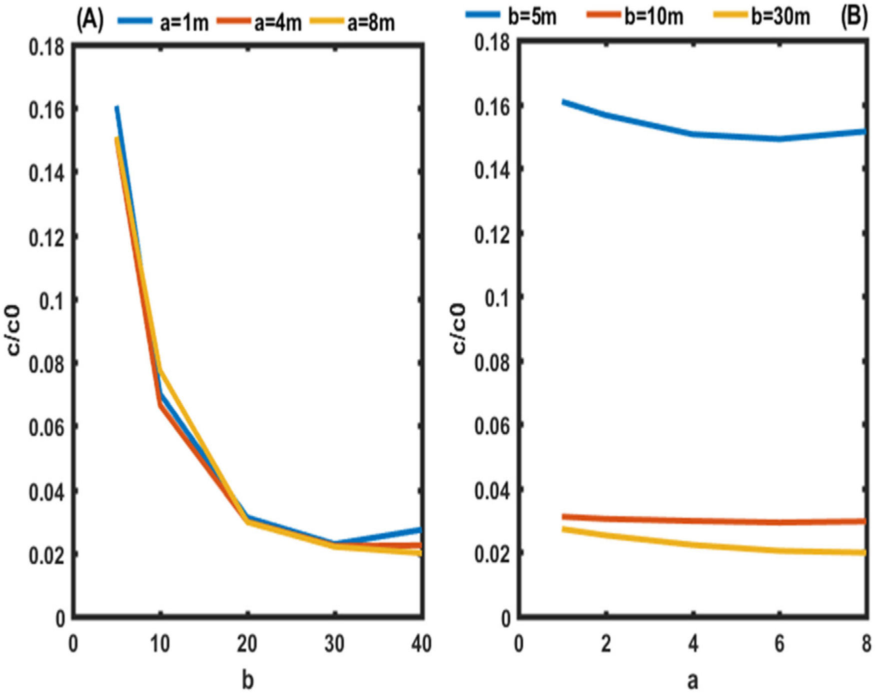

Figure 6. Behavior of pollutants at the outlet of the aquifer (0.9L) for the second condition. In In (A) the behavior of pollutants is given in function of b. (B) the behavior of pollutants is given in function of a.

for b = 40 m, the order of these positions becomes x/L = 0.28; 0.21; 0, 17 respectively for a = 4 m, 6 m, 8 m. These positions decrease with *a* an increase in the value of *b*.

Figure 8 keeps the same behaviour as Figure 7 with the only difference that the results are different at the outlet of the aquifer due to the boundary condition imposed at the other end of the aquifer. This work revealed that the adsorption and transport of pollutants in heterogeneous underground environments are improved when the value of the parameter b increases. Thus, b has a strong effect on the transport of solutes in the aquifer. However, Williams et al. (2003) have demonstrated the significant effects of pH and temperature on transport through porous columns. Natural phenomena (precipitation and climate change) also influence the parameters of the subsoil (Vengadesan and Lakshmanan, 2019).

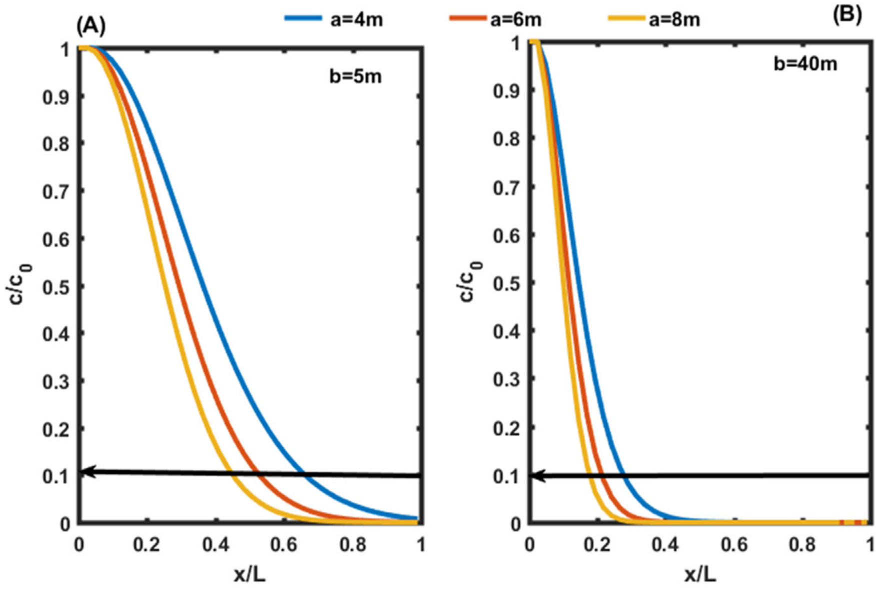

Figure 7. Concentration distributions as a function of distance at t = 50 days and v = 0.8m/day, for the first condition. In (A) the Concentration distributions is given for b = 5m. In (B) the Concentration distributions is given for b = 40 m.

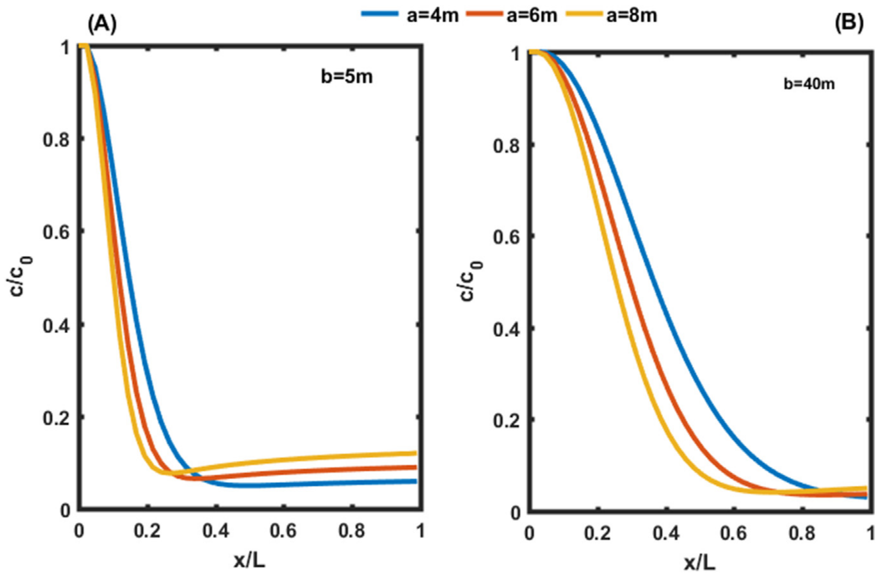

Figure 8. Concentration distributions as a function of distance at t = 50 days and v = 0.8m/day for the second condition. In (A) the Concentration distributions is given for b = 5m. In (B) the Concentration distributions is given for b = 40 m.

4. Conclusion

Groundwater is recognized as an economic resource and an ecological heritage that is important to manage and preserve. This is greatly important for a country located in coastal areas where the water requirements (irrigation and industry) are mainly groundwater. This article proposes the numerical resolution of the unidimensional advection-dispersion by the implicit finite difference technique method. The effect of dispersion, function of the distance of the transport of solutes in a porous medium has been analyzed for different boundary conditions at the outlet of the aquifer and for different dispersion parameters considered. The impact of the dispersion coefficient varying with respect to the depth of pollutants filtration in the sub-surfaces has been evaluated. It has been observed that the concentration of pollutants in the aquifer is influenced by various boundary conditions. The dispersion parameter b has an important effect on the transport of solutes in the aquifer more than the parameter, a. In other words, the mass of the retained solute increases with parameter, b. Nevertheless, in experimental conditions, some factors such as pH and temperature could have significant effects on the transport through porous columns. These conditions will be considered in future works.

Conclusion point-wise

- The effect of dispersion, function of the distance of the transport of solutes in a porous medium has been analyzed for different boundary conditions at the outlet of the aquifer and for different dispersion parameters considered.
- It has been observed that the dispersion parameter b has an important effect on the transport of solutes in the aquifer more than the parameter, a.

- The mass of the retained solute increases with parameter, b.
- Future works is focused on some factors such as pH and temperature to evaluate their effects on solute transport through porous columns.

Declarations

Author contribution statement

Calvia Yonti Madie: Performed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Fulbert Kamga Togue, Paul Woafo: Conceived and designed the experiments; Analyzed and interpreted the data.

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Data availability statement

Data will be made available on request.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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