New Trends in Groundwater Contaminant Transport Modelling

Kamilia Hagagg

Abstract Water is one of the essential interactive environmental and vital components for sustaining life on Earth. The increasing awareness about our environment and the recognition of the need for its protection support rational and efficient use of water resources planning qualitatively and quantitatively. In this context, using numerical models as a tool for diagnosing, managing, and predicting groundwater behavior has been gaining considerable importance in recent years. The study of solute transport related to groundwater contamination has become the focus of numerous researchers from many viewpoints, and the resulting achievements are so scattered and extensive. Therefore, this work documents various literature to systematically study the available theoretical and experimental works on groundwater contaminant transport modelling. Here, a simplified systematic and integrative picture of the present status of groundwater contamination is provided to emphasize the new trends and challenges to facilitate future research directions for more comprehensive analyses of the solute transport phenomena, with some recommendations toward solving these challenges.

Keywords Groundwater · Pathways · Contaminants transport modelling · Groundwater contaminants · Challenges in transport modelling

1 Introduction

Water is a vital key component in the development of nations. The efficient use of water resources has become important in future planning especially in arid African regions. In general, groundwater simulation models are mainly used for predicting the changes in groundwater level or in concentration, to test aquifer sustainable use or as protection strategies. In addition to hindcasts concentration changes, to determine the source of contamination or to design a proper monitoring network. The measurement

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of groundwater flow and pollutant transport is a challenging issue; hence the system of groundwater is dynamic one; predicting groundwater flows and contaminants transport through it is difficult. The characteristics that control groundwater flow and transport in an aquifer include those related to fluid and porous media properties are heterogeneous on large scales (e.g., porosity, permeability, storativity, dispersivity etc.). To simulate these intricate and sophisticated groundwater flow and transport phenomena, numerical models are necessary.

With growing awareness of the importance of protecting our environment, the study of solute transport related to groundwater contamination has become a primary focus for many researchers globally [9, 10, 23, 33, 37–39, 49]. Numerous researchers tried to solve the problem from different perspectives, and the resulting accomplishments are so diverse and dispersed that it appears necessary to inventory the completed works.

This chapter presents a systematic examination of the theoretical and experimental works that are currently available. A comprehensive picture of the problem's current state is also provided. Issues such as uncertainty, verification, and validation of the model output that are still unclear or unaddressed by recent researchers are highlighted to facilitate future research directions for a better understanding and more comprehensive analyses of the solute transport phenomena related to contaminate transport modelling. The chapter aims to identify and elucidate potential sources of contaminants water. In addition to examination of the progress made so far in using dispersion models in order to highlight the key issues and challenges confronting dispersion modelers. Also, it aims to identify future prospects and summarize the key areas requiring additional research to close evidence gaps and improve model performance.

2 Contaminants Sources and Their Pathways to Groundwater System

Any significant physical, chemical, biological, or radiological substance or matter that has a negative impact on air, water, soil, or living organisms is considered as an environmental contaminant, Shane [66] and Jaiswal et al. [41], WHO [80], Zhou et al. [85], Tokatli et al. [73] and Jabbo et al. [40]. Groundwater contaminants come from two categories of sources: point sources and non-point sources (distributed). Landfills, leaking gasoline storage tanks, leaking septic tanks, and accidental spills are examples of point sources. Infiltration from farmland treated with pesticides and fertilizers is an example of a non-point source, [18] as following.

Non-Point Source

- Fertilizers on agricultural land
- Pesticides on agricultural land and forests
- Contaminants in rain, snow, and dry atmospheric fallout.

Point Source

- On-site septic systems
- Leaky tanks or pipelines containing petroleum products
- Leaks or spills of industrial chemicals at manufacturing facilities
- Underground injection wells (industrial waste)
- Municipal landfills
- Livestock wastes
- Leaky sewer lines
- Chemicals used at wood preservation facilities
- Mill tailings in mining areas
- Fly ash from coal-fired power plants
- Sludge disposal areas at petroleum refineries
- Land spreading of sewage or sewage sludge
- Graveyards
- Road salt storage areas
- Wells for disposal of liquid wastes
- Runoff of salt and other chemicals from roads and highways
- Spills related to highway or railway accidents
- Coal tar at old coal gasification sites
- Asphalt production and equipment cleaning sites.

There are several pollution sources that pose risks to groundwater globally. Municipal landfills and industrial waste disposal facilities are two of the more important point sources in sand and gravel shallow aquifers at arid and semi-aridness. Under the risk of more extensive contamination might be enhanced. Septic tanks, petroleum product leaks and spills, and heavy industrial organic liquids are also a few of these risky and common causes of pollution. Bacteria, viruses, detergents etc., are some of the contaminants that can come from septic systems and infiltrate groundwater.

On the other hand, iron, manganese, arsenic, chlorides, fluorides, sulphates, and radionuclides are a few examples of naturally occurring materials that can occur in groundwater [2]. Particles from other naturally occurring substances in our environment, like decomposing organic matter, can migrate through groundwater. The migration of contaminates is mainly controlled by the surrounding environmental condition, such as, soil pH, redox conditions, biotic action, and the amount of water percolating the soil. When taken in large quantities, some pollutants can be harmful to the health. Unless it has been treated to remove the contaminants, ground water that has unacceptable levels should not be utilized for drinking water or other domestic water usage.

The first step is to fully understand groundwater flow and transport processes, taking into account critical parameters such as contamination activity location, intensity, and duration. The establishment of a proper flow and transport model ensures that the correct spatial and temporal distribution of contaminant concentrations is maintained throughout the site. The combined processes of advection and dispersion cause groundwater to move from higher hydraulic head towards areas of lower hydraulic heads, transferring dissolved solutes as well as contaminants. Advection describes the large-scale transportation of solutes by flowing groundwater. Dispersion is the process by which a pollutant plume moves from an area with a high concentration to one with a lower concentration. The advection–dispersion-reaction equation, which describes solute transport in many groundwater transport models, can be used to compute the dispersion coefficients as the total of mechanical dispersion, molecular diffusion, and macro-dispersion.

3 Numerical Modelling of Contaminates Transport

Although groundwater models are a simplification of a more complicated reality, they have consistently been effective tools for addressing a variety of groundwater issues and assisting in decision-making over several decades [44]. Any computer technique approximating an underground water system is known as a numerical groundwater model [5]. Numerical groundwater simulation models have developed into a promising technique in science and engineering during the last few decades for describing, evaluating, and evaluating physical systems and phenomena [44]. Hence, analytical solutions were insufficient to accurately characterize a subsurface system, as a results of the system's inherent heterogeneity; groundwater simulation models have been used to describe hydrologic phenomena to evaluate or forecast the long-term effects of water withdrawals and to investigate different groundwater management options, movement of water and oil in the subsurface, and movement of contaminants in the fields of groundwater hydrology with the goal of identifying a contaminant source and its plume extent. In numerical simulation models; a numerical simulator converts one or more partial differential equations converts one or more partial differential equations into a set of algebraic equations that can be solved for discrete values of the dependent variables. The models are separated into five groups [44] according to the numerical approach taken to solve these equations as following.

1. Finite differences.
2. Finite elements.
3. Integrated finite differences.
4. Boundary elements.
5. Analytical elements.

The most often used techniques for resolving groundwater flow and mass transportation issues are finite differences and finite elements. The collections of algebraic equations (system equations, boundary conditions, and initial conditions) that result from approximating partial differential equations are solved by a computer programme.

A simple protocol for groundwater modelling can be explained that starts with the planning of project problems, or phenomena to be modeled and also the selection of the used model. After that the conceptualization of the modeled system starts. The development of a valid conceptual model is the most important step in a modeling study after the definition of the study objectives, model purpose, and complexity at the scoping stage. A conceptual model is a simplified representation of the physical system's key features and hydrological behavior.

It serves as the foundation for the site-specific computer model; it is subject to some simplifying assumptions. The assumptions are necessary partly because a complete reconstruction of the field system is impossible and partly because there is rarely enough data to fully describe the system. The conceptual model must include all features that are relevant to the problem and the boundaries geometry of the investigated aquifer domain; it should specifically include the following.

- The aquifer matrices structure, homogeneities, and heterogeneities.
- The flow mode and regime in the investigated area.
- The properties of the water (homogenous, viscous, etc.).
- Sources and sinks of water and of relevant contaminants within the domain and their specific geometry.
- Initial conditions within the considered domain; across its boundaries.

The reliability or accuracy of the model is tested in the calibration step, in which the model reproduces or matches historically observed data (hydraulic head) [82]. Based on the results of this step, the key groundwater parameters are then modified and refined. A trial-and-error approach can be used for this process until a satisfactory match to observations is attained. Verification is the process in which the calibrated model can reproduce a set of field observations independent of that used in the model calibration (if they exist) [7]. The sensitivity analysis could be demonstrated through varying inputs over a reasonable range, within uncertainty in the parameter value, and observing the relative change in the model response. The sensitivity of one parameter versus others is also can be evaluated [5].

Now finally, the model can be used to predict the response against future scenarios after completing the calibration process, sensitivity analysis, and field verification. The estimation of the future hydraulic response of a region is important for protection, mitigation, and adaptation to any expected adverse effects [8].

4 New Trends in Groundwater Contamination Modelling

Groundwater contamination risk assessment offers a means for decision support through carefully assessing and ranking the severity of site contamination, helping identify critical issues for mitigation actions [12, 47]. Risk assessment is usually based on using mathematical models by predicting subsurface contaminant behavior into the future [16], although the efficiency of the mathematical modelling efforts usually requires sufficient knowledge of the subsurface hydrogeological conditions throughout a contaminated site. However, this knowledge is often limited by various uncertainties associated with soil and contaminant properties, and the risk is thus inherently linked with uncertainties [35]. It is recognized that the success of contaminated site risk assessment depends significantly on whether the contaminant transport and fate models have appropriately quantified and incorporated the related uncertainties into the simulation processes [48, 53]. Also, source identification and characterization can be more difficult for groundwater than for other environmental pathways. Several factors; the pollution sources' characteristics are difficult to measure due to several factors. Pollution sources that are only present in very small quantities might pose a potentially great health risk, depending on the toxicity of the substances.

4.1 The Remediation of Contaminated Sites

Once contamination has been detected in the subsurface, the pathways and fate of the contaminants must be predicted. This action should be taken as a mandatory response to any plan of mitigation, cleanup operations, or control measures toward planned remediation activities. Similarly, any monitoring or observation network should be based on the anticipated behavior of the system. There are two main strategies: (i) to hinder, modify or remove the migration of the contaminant from the source to the environment [1, 15, 61, 65]; or (ii) to protect the recipients from contamination by filters, barriers or pumping [13, 14, 72]. New techniques are continuously being developed to manipulate the contaminant source, but the latter strategy may be necessary for non-point sources as well as for contaminant plumes that have migrated long distances in the subsurface. When groundwater is used as a supply of drinking water, the management of an artificial aquifer recharge has also proven to be successful in meeting the standards for drinking water quality [30, 34, 70]. However, because of the heterogeneous conditions of the subsurface and the contaminants' adherence to soil particles, there are arguments that once an aquifer has been contaminated, it is difficult, if not impossible, to restore it to its original state [74].

4.2 Vadose Zone Contaminant Transport

The numerical problem for predicting contaminant transport in the vadose zone and in groundwater often becomes extremely demanding of computational power. A literature survey indicates that there has been an increasing tendency for numerical problems to be solved on networks of computers, which are not publicly available. Several studies were implemented on the effectiveness of aquifer remediation [52, 54, 58, 59]. They functioned their studies merely as demonstrators for specific numerical methods, simulators, or various remediation techniques. Therefore, an important research challenge is to focus more broadly on integrating appropriate methodological developments with the realities of field observations at specific sites to help solve real problems of the subsurface environment [31, 37].

4.3 Environmental Isotopes Hydrology

Recent research in this field [33, 55, 64], followed an attempt that used an integrated approach of the hydrogeological setting and the conjugation of the hydrogeochemical data with the stable isotope hydrology for representation of the conceptual model of the modeled area. Those tools give more insights into the characterization of the groundwater system with all relevant boundaries and main recharge sources of the aquifer, which is considered to be the key components in the groundwater modeling process.

4.4 Geochemical Modelling

Many studies combined two approaches to analyzing groundwater quality data: geochemical modeling of concentration profiles [6, 77] and trend detection concerning travel times. Many studies argued the geochemical modelling of nitrate and sulfate concentrations along the vertical component of groundwater flow within the studied aquifer. A notable effort has been made to improve the modelling of the transport and fate of contaminants by coupling transport models with geochemical models [17, 26, 49, 52]. Geochemical models essentially solve various chemical reactions based on mass conservation and chemical equilibrium principles with the aid of thermodynamics. Some of the geochemical models, such as MINEQL, EQ31EQ6, and MlNTEQ, also calculate adsorption/desorption and precipitation/dissolution. For example, the transport model, EXAMS, was coupled to MlNTEQ to form the model MEXAMS, which calculates chemical species of heavy metals, the amounts of adsorption/desorption and precipitation/dissolution, and the migration of heavy metals [43, 46, 81].

4.5 Mining Activities

The primary possible environmental sources of pollution at mining sites are rock waste materials and tailings, which interact with rain and leach into the aquifer. When exposed mining is completed, nature begins to re-establish the basic groundwater and surface water regimes, and the mine floods. Flooding creates pools at lower elevations, causing mine water quality to deteriorate. Groundwater modelling can provide on-site characteristics of the subsurface contaminant source in abandoned mine sites, as well as help to reduce uncertainties that govern groundwater flows and contaminant transport, as well as the most likely location and magnitude of the unknown contamination source. Under these conditions, the MODFLOW (flow) and PHT3D (reactive transport) simulation codes are widely used to predict spatial and temporal flows, as well as the concentration values in a contaminated aquifer [21].

4.6 Seawater Intrusion Studies

In the last decade, there were several density-dependent simulation codes developed based on the commonly-used groundwater model [68], among them, SEAWAT [29], which uses a modified version of MODFLOW [51] to solve the variable density groundwater flow equation and MT3D module [83]. Hagagg [31] and Hussien et al. [38] assessed the lateral extent of the seawater intrusion to predict the future behavior with respect to different stressing scenarios, many researchers used the SEAWAT code, as a useful tool for simulating three-dimensional variable-density groundwater flow.

4.7 Groundwater Management and Sustainability Studies

Management means making decisions to achieve goals without violating specified constraints. Groundwater sustainability was defined as "the development and use of groundwater in some way to meet the needs of present and future demand without causing unacceptable environmental, economic or social consequences" [4]. All such predictions can be obtained within the framework of a considered management problem by constructing and solving mathematical models of the investigated domain and of the flow and solute transport phenomena that take place in it. The determination of groundwater sustainable yield requires providing an optimal and quantitative outcome based on groundwater flow and mass balance principles. Much effort through research has contributed to studies on the definition, methods and factors of sustainable yield, either on an aquifer scale or a basin scale [3, 24, 36, 50, 76, 78, 84]. As a result of some difficulties in the conceptualization of the subsurface aquifer media and because models are often used to physically simplify a complex system and mathematically represent key phenomena of the system [19]. Various models have become the tools employed to understand groundwater systems via simulating and predicting its behavior [79]. Compared with analytical methods, numerical modelling provides a fast and sometimes effective way to evaluate groundwater resources' bulk behavior and quantity [27, 32, 62, 69].

4.8 Data Mining Algorithms

The main aim of using contaminant transport modelling is to understand the contaminant plumes' development and quantify the impacts to water quality. Data mining has recently considered the state of the art in different science applications dealing with large databases. Gaussian Process (GP) were used to predict nitrate (contaminant) and strontium (potential future increasing) concentrations in groundwater using various groundwater quality potential variables such as Temperature, pH, EC, HCO_3^-, F, Cl, SO_4^{2-}, Na^+, K^+, Mg^{2+}, and Ca^{2+} [11]. Different quantitative criteria, as well as a visual comparison approach, were used to assess the modelling capability in this study revealing that the GP algorithm outperforms all other models in predicting nitrate and strontium concentrations, followed by RF, M5P, and RT, respectively, according to the model evaluation criteria. This approach might present a new vision of using a large data set of specific contaminants with different mathematical algorithms to have a predictive future holistic picture of the status and concentration of contaminants.

In addition to that, Artificial Neural Networks (ANN) have recently been used in groundwater management to predict the hydraulic head at a well location and to simulate spatiotemporal groundwater levels [20, 25, 45, 56, 57, 71, 75]. ANNs mimic the hydraulic head using a black box method, incorporating hydrological data like rainfall and temperature as well as hydrogeological ones like pumping rates from neighboring wells. The network is trained using available field data, and the training process is assessed.

4.9 Stochastic Multicomponent Reactive Transport Modelling

In recent years, multicomponent reactive transport modeling (MRTM) has been used specifically to elucidate and simulate the controls of some contaminants to assist decision-makers in quantifying the potential extension contamination in aquifers [22, 26, 42]. Stochastic MRTM are useful tools for estimating the probability of non-exceedance (PNE) of a toxic aquifer compound in the presence of uncertainty [22, 63]. Model input parameters are treated as random spatial functions in stochastic analysis, while model outputs are expressed in terms of probability density functions. These functions' statistical indicators are used as metrics to quantify one or more desired target variables (e.g., the concentration of a polluting aqueous species), [60]. On the other hand, the empirical uncertainty caused by the incomplete mapping of the geochemical initial conditions (GICs) is a critical limitation for the MRTM predictions' reliability, Dalla Libera et al. [22]. When a system is out of chemical equilibrium, its initial geochemical status changes over time due to flow, transport, and geochemical transformations. Setting the correct GICs in each model cell is critical for correctly computing the PNE of a desired toxic compound.

5 Advanced Models in Groundwater Contaminant Transport

Several models were used for the predication and demarcation of contaminated plumes in groundwater systems. Some of them are mentioned in (https://www.epa.gov/land-research/ground-water-modeling-research), see Table 1.

Table 1 Some groundwater contaminant transport prediction models

Model	Specification
3DFATMIC	It simulates subsurface flow, transport, and fate of contaminants that are undergoing chemical or biological transformation. The model is applicable to transient conditions in both saturated and unsaturated zones. This model can almost eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective transport
3DFEMWATER/ 3DLEWASTE	They are related and can be used together to model flow and transport in three dimensional, variably-saturated porous media under transient conditions with multiple distributed and point sources/sinks. These models can be used to apply the assimilative capacity criterion to development of wellhead protection areas
BIOCHLOR,	It is a screening model that simulates remediation by natural attenuation of dissolved solvents at chlorinated solvent release sites. It includes three different model types: Solute transport without decay, solute transport with biotransformation modeled as a sequential first-order decay process, and solute transport with biotransformation modeled as a sequential first-order decay process with two different reaction zones
FOOTPRINT	It is a screening model used to estimate the length and surface area of benzene, toluene, ethylbenzene, and xylene (BTEX) plumes in groundwater, produced from a gasoline spill that contains ethanol
Modular 3-D multi-species transport model (MT3D)	It is a 3D solute transport model for simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems. The model uses a modular structure similar to that implemented in MODFLOW
Nonaqueous-phase liquid (NAPL) simulator	It conducts a simulation of the contamination of soils and aquifers that results from the release of organic liquids commonly referred to as nonaqueous-phase liquids (NAPLS). The simulator applies to three interrelated zones: a vadose zone in contact with the atmosphere, a capillary zone, and a water-table aquifer zone
WhAEM2000	It is a public domain, groundwater flow model designed to facilitate capture zone delineation and protection area mapping in support of the State's Wellhead Protection Programs (WHPP) and Source Water Assessment Planning (SWAP) for public water supplies in the United States. It provides an interactive computer environment for design of protection areas based on radius methods, well in uniform flow solutions, and hydrological modeling methods

6 Challenges in Groundwater Contaminants Modelling

Most natural groundwater systems exhibit significant heterogeneity in aquifer system that affects on its physical and chemical properties. Groundwater management modelling is hampered by such heterogeneities [67]. There can be no "optimal" management strategies if the aquifer simulation model cannot be reliably calibrated. In fact, regardless of how thoroughly a simulation model is calibrated, there is always some degree of uncertainty in both model input and output. Furthermore, significant uncertainties are always present in economic and policy factors. Thus, since groundwater management modelling became an active field of research, how to adequately accommodate uncertainties in simulation and economic models has long been a focus point. As groundwater management modelling becomes more sophisticated, this topic is likely to remain a major focus of future research. Nevertheless, since there is no other way but to use models in order to predict the future behavior of an investigated system, using whatever data that are available for model calibration (despite of the associated uncertainty). So, a strong monitoring approach to validate and track outcomes is vital and mandatory.

Groundwater management modelling has mainly focused on incorporating simulation with optimization methods to investigate critical issues ranging from contaminant remediation to agricultural irrigation management [28]. Still the broad impacts of global change on aquifer storage and depletion trajectory management that are defendants on surrounding environments need more enhancements. The scope of research efforts is only beginning to address complex interactions using multiagent system models that are not easily formulated as optimization problems and consider a variety of human behavioral responses.

Stochastic MRTM have not been widely used so far as a result of very long computational times regarding solving the nonlinear equations characterizing this type of model, in addition to the number of unknowns and input parameters required to run MRTM.

7 Conclusion

Groundwater flow and solute transport modeling is a vital and mandatory water management tool. It represents a simplified version of the real field site, helping understand the system and predict its behavior. The main goal of modelling in the groundwater field is to predict the value of an unknown variable such as head in an aquifer system or the concentration distribution of a chemical in the aquifer in time and space and predict the future changes of the system. Detection of groundwater contamination is considered to be a vital importance to manage and protect groundwater from anthropogenic pressures. This review introduces a special focus review for modelling the contaminant transport starting from the occurrence of groundwater contaminants including natural and anthropogenic, their movement, mathematical modelling, and recent trends in this topic. It was revealed that till now, issues such as heterogeneity of the modeled system, uncertainty in model input, and limitation of the available data describing the underground system are complicating the accurate estimation. In general, modelling of contaminants' transport in the groundwater system using a real-world simulation has been improved compared to earlier attempts to calibrate a simulation model for the complex flow and transport process. Although, recently, the application of data mining in filling the unknown gaps in modeled information seems to be promising. In addition to the application of data mining in forecasting and prediction problems as hydraulic head might be extended in the future for predicting the behavioral attempt of contaminated plumes.

8 Recommendations

1. Putting more strategies in accurately selecting the model inputs is one of the most important factors that might reduce uncertainties in the output of numerical models.
2. Integrating some advanced models as data mining in predicting attributes and data in unreached areas to facilitate the conceptualization process prior to modeling.
3. Conjugation of several models might compensate for the data gap and decrease the uncertainty of the modelling process.
4. Linking the solute transport in unsaturated zone with subsurface groundwater flow and mass transport might help in knowing the behavior of the contaminants in these zones and hence mitigate their plumes.
5. It is mandatory to trace and link the climatic change on the behavioral of the aquifer response and quality aspects.

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