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A Multi-Phase Flow Model for Predicting Contaminant Transport in Underground Aquifers

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Abstract:
The threat of groundwater contamination is great to our most precious resources on this planet. Urban development and industrial activities are encompassing the entire globe and need for accurate model to predict and mitigate the transportation of pollutants in underground aquifers is becoming important day by day. In this article progress is made for the development and use of multi phase flow models for predicting transport of contaminants in subsurface environment is explored, by highlighting major advances and scope for further research. Extensive research of the complex interactions between contaminants and aquifer systems has arisen from the growing concern over the quality of groundwater. Powerful tools for simulating movement of different fluid phases such as water, air, and organic pollutant through the porous media include the multi-phase flow models. Such models can be used to gain valuable information about how contaminants may be fated and transported and provide an impetus for development of more effective remediation strategies and better decision making in environmental management. In this extensive exploration of multi phase flow models, we present an introduction of fundamental principles governing multi phase flow models, assess their development over the past few decades and discuss their use in predicting contaminant transport. This paper synthesizes previous studies that address specific workings of multi-phase flow modeling in the field of groundwater contamination and it aims to facilitate understanding of the present state of the task by identifying research areas in the future.

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1. Fundamentals of Multi-Phase Flow in Porous Media

The study of multi phase flow in porous media plays an important role in hydrology, environmental engineering, and petroleum engineering for they determine the movement and distribution of several phases (water, air, oil, and gas) within the pores of the geological formation like aquifers, reservoir, soil. Accurate prediction of behaviour of contaminants in the groundwater, oil recovery processes and subsurface fluid management requires the understanding of multi-phase flow. In comparison to single phase flow, which usually involves only one fluid (typically water), multi phase flow happens when two or more immiscible fluids move simultaneously through the portion of the pore space.

The flow behavior of each phase is determined to some degree by interactions between phases and the solid matrix of the porous medium. For the fluids to flow through the porosity, the media's porosity and permeability are very important in defining the ease with which each fluid can pass through the pores. The fraction of void space occupied in the porous medium that stores fluids is porosity, whilst the permeability of the medium as a measure of the ability of the fluids to flow within it. The relative permeability of each phase to a given flux depends upon that phase saturation and carries the major dependence of its physical nature as a multi phase flow [1]-[4].

Capillary pressure is one of the fundamental principles of governing multi phase flow; it is the difference of the pressure between the two immiscible fluids at the interface in porous medium. This arises in consequence of the surface tension between the phases and the solid boundaries of the pores. Capillary pressure affects the distribution of each phase in the medium and, especially, the relative flow behavior of the fluids in aquifers and reservoirs. In the wetting phase (usually water under unsaturated condition), the surface of the porous material is more wetted, and the non-wetting phase (e.g. oil or gas), is pushed back inside the pores by the wetting phase into disconnected clusters.

Darcy's Law accounts for multi phase flow dynamics but it has also been extended for more than one phase. Darcy's Law has an extended form that takes a flow rate of each phase as a function of the pressure gradient, the permeability and the relative permeability of each phase. Relative permeability is the measure of the ratio of the flux of a certain phase, through a matrix, divided by the total permeability that the matrix can provide to all phases. Saturation related variation is different, and is controlled by interfacial interactions between fluids [5]-[8].

The saturation and distribution of each phase in a multiphase system can be classified in different flow regime. For example, if a water-oil system has high water saturation, then the flow is practically all governed by the water phase and the oil phase is compromised to fixed pockets or films. On the contrary, in the situation where oil saturation is greater oil will govern the flow, while water is dispersed in isolated portions. The system will shift between these modes with respect to the mobilities and saturations of the phases present [9]-[14].

Table 1: Model Parameters for Multi-Phase Flow Simulation

Parameter	**Unit**	**Description**
Porosity	–	Fraction of pore volume in the aquifer
Permeability	m^2	Intrinsic permeability of the porous medium
Viscosity (water)	Pa·s	Dynamic viscosity of water
Viscosity (non-aqueous phase liquid)	Pa·s	Dynamic viscosity of NAPL
Density (water)	kg/m^3	Density of water
Density (NAPL)	kg/m^3	Density of the contaminant phase
Longitudinal dispersivity	m	Controls solute spreading along flow path
Transverse dispersivity	m	Controls solute spreading perpendicular to flow
Partition coefficient	m^3/kg	Governs equilibrium sorption of

(sorption)		the contaminant
Retardation factor	–	Delays solute movement due to interaction with solids

Multi phase flow models are used to simulate and predict the behavior of fluids in the porous media by solving the governing equations which includes the interaction of phases. These models described by mass balance equations as each fluid phase in the system is conserved. Mobility ratios are included as they represent the relative ease with which each phase can move through the medium under current prevailing pressure and saturation conditions. Often the equations described above are solved numerically in complex, heterogeneous media with analytical solutions difficult to obtain; numerical methods such as finite difference and finite element techniques are frequently employed.

Multi phase flow models are important when it comes to understanding the way in which contaminants (such as oils, chemicals, and other 'contaminants') flow in the groundwater system. Predicts the mechanisms by which contaminants interact with each other, as well as with water and other immiscible phases present in the subsurface, and how they will be acted upon by capillary forces, pressure gradients and changes in porosity and permeability induced by geological heterogeneity. Managing groundwater resources, mitigating pollution, and optimizing techniques for oil recovery depend on an understanding of the multi phase flow behaviour.

The second conclusion relating to the concept of multi phase flow in porous media is that it is a complex and important concept, defining transport and distribution of multiple phases of the fluids within the pore structure of natural and engineered systems. Simulations are able to better understand the interaction between phases and accurately predict the behavior of fluid in applications such as groundwater contamination to petroleum extraction through the application of advanced models and simulation techniques [16]-[19].

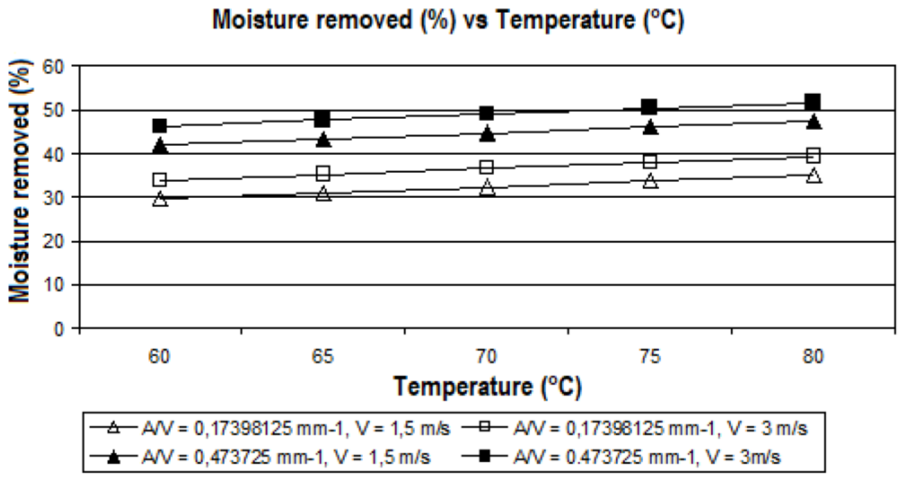

Fig. 1. Historical Development of Multi-Phase Flow Models

2. Early Approaches

Multi phase flow in porous media is studies in petroleum engineering where the goal was to understand, and optimise oil and gas recovery processes. Initially, early models were based on simplified representations of two phase flow; for instance oil and water as the considered principal fluid phases.

These concepts were adapted to environmental applications in the 1950s and 1960s when researchers began developing multi-phase flow models for the movement of contaminant in groundwater systems. They were the beginnings of models that would come to be a lot more sophisticated in the decades to come [20]-[23].

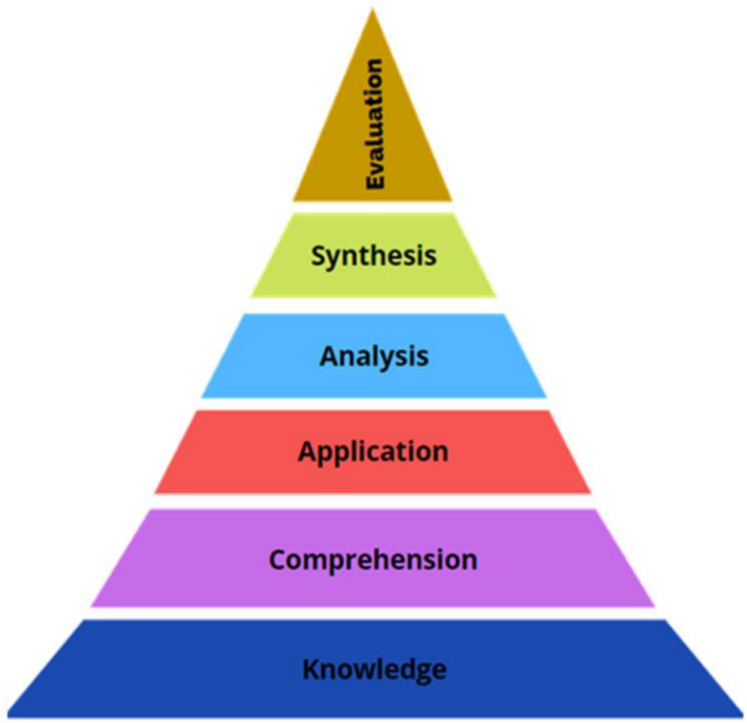

Fig. 2. Our models are based on key components of Multi-Phase Flow Models.

Multi phase flow models are useful tools to explore the behaviors of multiple fluid phases moving through the porous media like in underground, oil reservoirs and other subsurface systems. They play a critical role in understanding how various fluids (e.g. water, oil, gas, and contaminants) in a medium will participate in transport, mix, and phases. These models would incorporate some key components to allow us to simulate and analyze multi phase flow accurately. The key components in capturing fluid dynamics complexities and ability of the models to make meaningful predictions in practical applications, including in environmental monitoring, petroleum recovery, and contaminant transport studies, are these.

The mass balance equation forms one of the basic part of multi phase flow model. This equation is intended to describe the conservation of mass for each phase in the system. The model guarantees that the mass that entered a control volume was balanced by the mass that went out of the volume and the mass accumulation in that specific volume for every fluid phase (water, oil, gas, etc.). More often than not, the mass balance equation is expressed as a partial differential equation where the variables of interest are pressure, fluid saturation, and velocity. These equations guarantee proper description of movement and accumulation of each fluid phase as it comes in contact with the working medium.

Another important component in these multi phase flow models is Darcy's Law. The extended version of Darcy's Law describes the flow of each of the fluid phases through porous media. It is a correlation between flow rate of each phase and pressure gradient permeability, and the relative permeability of phase. Relative permeability describes how the relative amounts that a phase will fill the pores of a rock as vs. the saturation of other such phases present in a system. The full form of Darcy's Law enables the simulation of movements of multiple phases in a single model where the movements of different phases are influenced by the relative permeabilities of these phases in relation to each other [26]-[29].

Capillary pressure appears to be an important concept in any multi phase flow model in which immiscible, or water and oil, is considered. The pressure difference (capillary pressure) between two phases i.e. water and oil at an interface within a porous medium is surface tension dependent and depends on geometry of the pore space. Capillary pressure has a large bearing on how fluids distribute themselves in the pores and thus how fluids might flow, especially in unsaturated conditions. Here it is particularly important, because it determines how one phase displaces another in the presence of pressure gradients, and consequently is very important for modeling contamination movement in groundwater or oil recovery in a reservoir.

An important part of it is the relative permeability function. The relative permeability is a measure of the ease of transport of each phase thru the porous medium in the days of other phases. As the saturation of one phase increases, the relative permeability of the other phase decreases, such that the other phase becomes less capable of permeating the medium as its saturating phase occupies a larger portion of the pore space. Use of this function is crucial to simulate real world flow circumstances where competition for the available pore space between phases happens and that have a powerful effect on flow rates and saturation distribution.

It is within saturation that the key variable of the models multi phase flow is, to represent the fraction of the pore space occupied by a given phase. The saturation is time dependent and has different spatial dependence across the porous medium. Flow equations for press, velocity and capillary forces govern the evolution of phase saturations. Fluid phases flowing through the medium experience changes to their saturations and must be simulated to correctly predict fluid distributions within the system [30]-[32].

Multi phase flow models are also characterized by flow regimes and phase interactions. The flow may switch between different regimes as the relative saturations of the phases and the conditions change in many porous media. To illustrate, the flow will transition from drainage (where the non wetting phase displaces the wetting phase) to imbibition when the water phase saturating increases. In order to understand the behavior of multi-phase systems under different conditions, it is essential to understand the flow transitions and accurately model the phase interactions.

Numerical methods and computational techniques are finally essential components to the solution of multi phase flow models. The multi phase interactions are of considerable complexity and the governing equations are highly non linear for which analytic solutions seldom exist. As a result, many multi phase flow problems are solved numerically using finite difference methods (FDM), finite element methods (FEM) and Smoothed Particle Hydrodynamics (SPH). Discretization of the problem domain leads to small elements or grid points, on which the governing equations are solved iteratively to the flow behavior of each phase for a certain amount of time.

Therefore, in conclusion, the mass balance equations, Darcy's Law, capillary pressure, relative permeability functions, phase saturation, and numerical solution techniques make up the important components of these multi phase flow models. Individual, to simulate complex fluid phase interactions in porous media, these components work together to predict fluid movement, transport and distribution accurately. Such models are key to a large number of applications, including environmental remediation, petroleum extraction and groundwater management, by allowing cost benefit optimization of processes and more intelligent decision making on managing multi phase fluid system.

3. Relative Permeability and Capillary Pressure Functions

Multi phase flow model requires relative permeability and capillary pressure functions for the interaction between fluid and porous medium. Usually, these functions depend on the saturation status of the corresponding fluid phases and they can vary greatly in a particular fluid-solid system under consideration.

The ability to accurately represent relative permeability and capillary pressure relationships is required for predicting phase distributions and flow behavior in the multi phase systems. Based on these relationships, researchers have developed a number of empirical and theoretical models for predicting them, the accuracy of which continue to be improved and the applicability extend to a variety of subsurface environments.

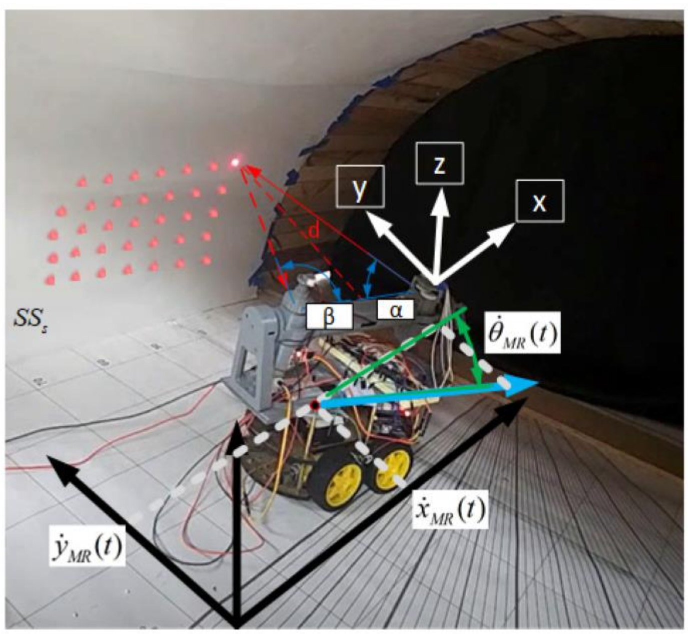

Fig. 3. Numerical Methods for Solving Multi-Phase Flow Equations

Solving complex partial differential equations (PDEs) describing the behavior of multiple fluid phases and interplay in the porous medium constitutes the real part of simulation multi phase flow in porous media. Typically, mass conservation, momentum conservation, energy conservation, together with their interactions, namely, capillary pressure, relative permeability, and fluid saturations are usually accounted for in these equations. Analytical solutions are not possible because of the non linearity and complexity of the multi phase flow problem, especially in real world problems. Therefore, these equations are approximated using numerical methods. Solutions to multi phase flow equations have been achieved by means of different numerical techniques that present their own advantages and disadvantages.

Finite Difference Method (FDM) is one of most widely used numerical methods to solve multi phase flow equations. Finite Difference Method is a technique of discretizing the continuous domain into a grid of points and approximating the derivatives in the governing equations using finite difference equation. Compared with other methods, this is a simple and easily applied procedure to simple geometries with uniform grids. Its usefulness is particularly significant in problems for which the governing equations are relatively simple (and exists at least one regular grid solution) for which it is desirable to study a range of parameters and phenomena. On the other hand, the solution details of complex geometries are often required using finer discretization using FDM, which can be computationally costly [33]-[34].

The Finite Element Method (FEM) is another commonly used numerical technique. FEM has been proved to be particularly efficient in solving complicated multi-phase flow problems in irregular geometry, for example, heterogeneous porous media. In FEM, the domain is broken into smaller subdomains or elements, in which the solution is approximated by using interpolation functions. The PDEs are transformed to an algebraic system of equations which are solved numerically by the method. The flexibility of FEM in handling complex boundary conditions and varying material properties allows it to make good use for the applications in environmental engineering, petroleum reservoir simulation and groundwater flow modeling. FEM however, does require large computing resources, especially for large scale problems with a need for a fine mesh along with a complex solver.

A second widely used numerical method for solving multi phase equations, for example computational fluid dynamics (CFD) and reservoir simulation, is Finite Volume Method (FVM). The control volumes in which the problem is discretized is done by FVM and then applied to conservation equations. On the other hand, the major advantage of FVM is its ability to conserve mass, momentum, and energy at each control volume that makes FVM ideal for simulation of the conservation laws in such fluid flow problems. FVM can also handle complex boundary condition since it is also flexible. It can be combined with other methods called FEM or FDM for better accuracy. The computational cost of FVM for high resolution simulation becomes significant in large scale multi phase flow problems because one needs to solve large system of equation.

Table 2: Simulated Contaminant Concentration Profiles Over Time

Time (days)	**Monitoring Point (m)**	**Water Saturation**	**NAPL Saturation**	**Contaminant Concentration (mg/L)**
0	10	0.95	0	0
30	10	0.92	0.03	12.5

60	10	0.89	0.06	32.7
90	10	0.85	0.09	48.2
120	10	0.83	0.11	58.9
150	10	0.8	0.13	66.1

Smoothed Particle Hydrodynamics (SPH) has become popular for more dynamic simulations involving large deformations or separations of different phases. The SPH is a mesh free, Lagrangian method where the fluid is represented by particles that have properties like mass, velocity and pressure. The system is solved according to the physics of the system, since the particles interact with each other and the flow properties are calculated based on interaction between neighbouring particles. SPH is especially suitable for problems with free surfaces, including fluid dynamics in porous media, where grid based methods face difficulties in tracking the interfaces. However, SPH can be computationally expensive for large systems as large number of particles are required to get reasonably accurate results [35].

Another numerical method that integrates both Eulerian and Lagrangian approach to solve a fluid flow problem is Particle-In-Cell (PIC). The PIC method is a fixed grid (Eulerian) solver of the governing equations and a Lagrangian tracker of the movement of particles. This method is particularly useful when dealing with multi-phase flow in porous media in which phase interactions play an important role, as in capillary driven flows and oil–water displacement problems. It provides flexibility in tracking interface between separate phases and can save computational cost on tracking interface in complex fluid behavior in porous media. Although, handling the accuracy of particle interactions and computational costs constitutes the challenge.

The other class of numerical techniques often used for modeling of multiphase flow such as in cases where stochastic processes (random pore structures or uncertain material properties) have a major role is known as Monte Carlo methods (MCM). In Monte Carlo simulations fluids are modelled in the porous medium by drawing multiple random samples. These methods are then employed to estimate averages or probabilities of particular kinds of outcomes here, for instance the movement of contaminant plumes in groundwater. While Monte Carlo methods offer flexibility in handling uncertainty and variability, they can also be computationally expensive and may be impractical since many simulations are often necessary to generate acceptable results.

Another type of mesh-free methods, such as Element Free Garmerkin (EFG) Method, is also widely gaining popularity in multi phase flow simulations. Many of these methods do not require a structured mesh and are thus suitable to simulate problems involving large deformations, fractures or complex fluid-structure interactions. In mesh-free methods, the continuum is represented by a set of particles and the solution is found by using shape functions defined over a set of neighboring particles. In multi phase flow problems they can deal with complex boundaries and interfaces such as the moving interface between two or more fluid phases.

4. Conclusion

With the development of modeling multi phase flow models, they have now become indispensable tools for predicting contaminant transport in underground aquifers and provide important information into the complex processes which dictates the fate of pollutants in subsurface environments. In this article we have discussed how these models have evolved dramatically over the past several decades, thanks to the advancements in our understanding of the underlying physical and chemical processes, and in the numerical methods as well as computational techniques used to evaluate them. Future challenges of groundwater contamination will be met through the continued development and application of multi phase flow models. The integration of new technologies such as machine learning and high resolution imaging techniques as well as coupling with reactive transport and biogeochemical models will enable researchers and practitioners to have a better understanding and be able to predict and mitigate the impacts of contaminants on our cherished groundwater resources. The future is looking to multi phase flow modeling for its ability to continue protecting and managing our underground aquifers. It is at the fore front to address current limitations and to embrace modern technologies to contribute immensely to environmental management and sustainable water resource practices in the future.

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