FVM for Solving Three Phase Percolation Model of Unsaturated-saturated Zone

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ABSTRACT: The petroleum leaking into the underground would threaten the groundwater systems. This is a complex water, oil, gas dynamic process of three-phase flow. Quantitative description of the spatial and temporal characteristics of the pollutants in groundwater numerical method for this kind of problem can provide scientific support and theoretical basis for oil pollution control. This dissertation describes water, oil, gas phase percolation model and Constitutive. For the multi-phase percolation model, since the finite difference and finite element method is not conserved, the author used the finite volume method. And using circumventers dual subdivisions and center of gravity discrete the three-phase seepage control equation dual subdivisions. It get a discretization scheme of Water, oil, gas phase on the dual unit control volume, which need a linearization by using IMPES and SS. In this dissertation, the finite volume method main advantage is the ability to handle complex grid, and meet the physical law of conservation. It is easy to set up conservation format. But discrete format is non-linear differential equations needing to rely complex constitutive relation, brought a certain degree of difficulty for the solution of the model. To verify the validity of the mathematical models and numerical methods, Example calculated the leakage of petroleum pollutants in the saturated zone - the unsaturated zone seepage law: oil leakage into groundwater slowly under the action of gravity downward expansion and to both sides of the penetration. With the years of growth, the petroleum pollutants saturation gradually reduces, but also brought to groundwater pollution.

1 INSTRUCTION

Petroleum products often use pipeline transportation and underground storage tanks storage, and due to external effects, there are often unexpected accidents, causing oil leakage and leaching, resulting in contamination of soil and groundwater. Its mechanism is complex, and it is a multiphase flow problem, that is, water-oil-gas phase coexistence state[Xue Qiang et al. 2002 & Smith D W et al. 1993]. To solve such problems, the numerical algorithm can be used to quantify the spatial distribution of petroleum pollutants in the unsaturated-saturated zone which can be effective in helping control of petroleum pollutants in groundwater pollution, to prevent causing more damage to the environment [Wang Hongtao et al. 2000].

Firstly, this paper introduces three-phase flow model and constitutive equations, and then solves the percolation model using numerical method. Commonly used numerical methods include Finite Difference Method (FDM), Finite Element Method (FEM) which have their own advantages and disadvantages. FDM is the earliest use of the numerical simulation method, because it is simple in form and relatively easy to calculate, but it has geometric error; approaches of processing boundary conditions are not uniform; and it is difficult to construct the high order convergence format. Basis of the FEM is the variational principle and the weighted residual method. It have many advantages such as strong adaptability, unified processing on boundary conditions, perfect theoretical basis, arbitrary grid discrete. However, it have many disadvantages either, like it can’t satisfy the law of conservation of mass; sometimes it can’t give a reasonable physical explanation; and the computation is large.

A new generation of numerical algorithm belongs to the Finite Volume Method (FVM) [Hunter, B. et al. 2016, Shewchuk, J.R. 2002, & Hejazi, H. et al. 2014] Its processes are that divide the solving area into a series of discrete non-overlapping control volume, and make sure each node has a control volume around; integral the differential equation to be solved at each little control volume to derive a set of discrete equations. The FVM requires solving the node value, which is similar to the FDM, at the same time; it must be assumed value distribution between
grid points within the integral equation, which is similar to the FEM. The advantages of the FVM are that its basic idea is easy to understand; it can draw a direct physical interpretation; and it satisfies the conservation of mass in space. In addition, the FVM’s mesh is flexible, theoretical basis are relatively prefect, and the amount of calculation is between the FDM and FEM.

2 MODEL INTRODUCTION

2.1 Control equations

According to the law of mass conservation and Darcy’s law, the continuity conservation equations of water (w), oil(o), and air(a) in a two-dimensional Cartesian area is as below[Kaluarachchi, J.J. & J. C. Parker 1989]:

\[
\frac{\partial \phi S_k}{\partial t} + \frac{\partial}{\partial x} \left( \phi K_u \left( \frac{\partial p}{\partial x} + \rho_p u \right) \right) + \frac{\partial}{\partial y} \left( \phi K_u \left( \frac{\partial p}{\partial y} + \rho_p u \right) \right) + \frac{R}{\rho_p} \frac{\partial \rho S_k}{\partial t} = 0
\]

(1.1 a)

\[
\frac{\partial \phi p}{\partial t} + \frac{\partial}{\partial x} \left( \phi K_u \left( \frac{\partial \rho}{\partial x} + \rho_p u \right) \right) + \frac{\partial}{\partial y} \left( \phi K_u \left( \frac{\partial \rho}{\partial y} + \rho_p u \right) \right) + \frac{R}{\rho_p} \frac{\partial \rho S_k}{\partial t} = \frac{p}{\rho_p}
\]

(1.1 b)

\[
\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x} \left( \phi K_u \left( \frac{\partial \rho}{\partial x} + \rho_p u \right) \right) + \frac{\partial}{\partial y} \left( \phi K_u \left( \frac{\partial \rho}{\partial y} + \rho_p u \right) \right) + \frac{R}{\rho_p} \frac{\partial \rho S_k}{\partial t} = 0
\]

(1.1 c)

In the formulas above, \( \phi \) is the porosity of the porous medium; \( S_p \) indicates \( p \)-phase saturation (\( p = \text{a(air)}, \text{o(oil)} \) or \( \text{w(water)} \)); \( x \) and \( y \) are Cartesian spatial coordinates; \( \rho_p \) is the density of \( p \)-phase; \( R_p \) is quality net transfer capacity of \( p \)-phase unite volume of the porous medium, with sign “(+)” (source) or “(-)” (sink); \( t \) represents time; \( K_p \) is the conductivity tensor of \( p \)-phase; \( \rho_{p} \) is the density of phase pressure; \( g \) is the acceleration of gravity; \( \rho_w^0 \) is the density of pure water; \( \rho_{pw} = \rho_p / \rho_w^0 \) represent \( p \)-phase bulk density; \( u_x = \partial z / \partial x \) , \( u_y = \partial z / \partial y \) denote the unit vector weight ratio, and up is positive; \( z \) is elevation. Besides, conductivity tensor can be transformed into a diagonal form according to the coordinate transformation, namely \( K_{xy} = K_{yx} = 0 \).

Formula (1.1) is established continuity conservation equations of multiphase flow model, in which three-phase saturation and head value is unknown.

2.2 Constitutive relation

The relationship among the pressure head, saturation and relative permeability is the most basic, the most complex but also the most critical parameters in the research of multiphase flow in porous media. It is often obtained by the experimental determination. Researchers is trying to mathematical descript the relationship of the parameter base on analyzing and comparing the influence factors of various parameters, which is also a necessary requirement for multiphase flow problems of numerical simulation[Wu Xiaofeng et al. 1999].

In the numerical calculation, the constitutive relation has the effect of the auxiliary system of differential equations. From the control equations (1.1), it is need to determine the relationship among saturation, pressure head, and relative permeability (S-P-K) [Kaluarachchi, J. J. et al. 1990].

At first, define the capillary pressure:

\[ h_{aw} = h_a - h_w; \ h_{ow} = h_o - h_w; \ h_{ao} = h_a - h_o \]

Among them, \( h_p = P_p / g \rho_w \).

The relationships of the three phase capillary pressure and saturation (P-S) are as follow:

\[ \overline{S_w} = [1 + (\beta_{aw} h_{aw})^m]^{-1}; \ \overline{S_{ow}} = [1 + (\beta_{ow} h_{ow})^m]^{-m} \]

And the relationships of the relative permeability and saturation (K-S) are as follow:

\[ k_{aw} = (\overline{S_w})^{1/2} [1 - (\overline{S_w})^{1/m}]^{1/2} \]

\[ k_{ow} = (\overline{S_{ow}})^{1/2} [1 - (\overline{S_{ow}})^{1/m}]^{1/2} \]

\[ k_{ao} = (1 - \overline{S_{ow}})^{1/2} [1 - (1 - \overline{S_{ow}})^{1/m}]^{1/2} \]

where \( \overline{S_w} \) is the apparent water saturation; \( \overline{S_{ow}} \) is the effective total liquid saturation; \( \beta_{aw} \) is the scale coefficient, which is approximated by the ratio of the surface tension of the water and the oil; \( \beta_{ow} \) is the scale factor, which is approximated by the ratio of the surface tension of the water and oil-water interfacial tension; \( k_{pw} \) is the relative permeability ratio of \( p \)-phase and water-phase.

3 FVM TO SOLVE THE MODEL

The first step in solving a numerical calculation of multiphase flow problem is to discrete the region, which will not be the rule in actual problem[Tao Wenquan 2001]. So this paper uses the circumcenter dual subdivision based on triangle subdivision (fig.1).
The figure is based on node-centric dual subdivisions, where $P_i$ is an adjacent node; $M_i$ is the midpoint of $P_0P_i$; $Q_i$ is the circumcenter of the unit $\Delta P_0P_iP_{i+1}$. So the polygon area that is composed by $M_1$, $Q_1$, $\cdots$, $M_6$, $Q_6$, $M_1$ is the circumcenter dual split unit $K^*_P$.

After discrete spatial region, we can discrete the differential equations. For the equations (1.1), this paper does integral respectively of the three-phase control equations in the unit time and the dual partition [L I Rong hua et al. 2000]. Then based on the Green formula and the properties of dual elements, simplify the integral equations. Processing method of the source and sink is to make them linearization. After that, we will get discrete equation group which is a nonlinear problem. Therefore, the next step is to make the nonlinear equations linearized base on the constitutive relation. Finally, the linear equations are solved by the SOR method.

4 AN EXAMPLE

4.1 Physical model

To validate the model and algorithms, and simulate the migration and distribution of the petroleum organic pollutants in unsaturated-saturated zone, this paper use a vertical cross section of multiphase flow model as an example. The following is a two-dimensional Descartes plane model with stable hydraulic gradient [A. K. Katyal et al. 1991].

The region is a rectangular area with 11m in horizontal and 8m in vertical, and the initial water head is at the bottom left border 4m and the right border of 3.5m. The bottom surface is a weak permeable layer, and the top surface is soil. The oil spill occurred in a strip area of 5m form the upper left edge of the top layer. And table 1 is list the medium and fluid properties.

<table>
<thead>
<tr>
<th>Medium Properties</th>
<th>Fluid Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{nw}$ = 10.0cm$^{-1}$</td>
<td>$\beta_{ow}$ = 2.69</td>
</tr>
<tr>
<td>$K_{nw}$ = 5.0cm$^{-1}$</td>
<td>$\beta_{ow}$ = 1.59</td>
</tr>
<tr>
<td>$\phi$ = 0.35</td>
<td>$n = 2.8$</td>
</tr>
<tr>
<td>$\phi$ = 0.05</td>
<td>$S_{ow} = 0.2$</td>
</tr>
<tr>
<td>$r_0 = 0.832$</td>
<td>$\alpha = 5.0m^{-1}$</td>
</tr>
</tbody>
</table>

4.2 Result

Fig 3 lists the oil saturation contour of different days after the oil spill.

![Figure 3(a) 10 days later, Oil saturation contour.](image)

![Figure 3(b) 50 days later, Oil saturation contour.](image)
It can be seen that after the leaking oil into the groundwater, it will slowly downward under the action of gravity, and due to the horizontal flow of water, the petroleum pollutants will permeate on both side. As the growth of the time, the pollutants did not enter the saturated zone, but caused the unsaturated zone pollution. Unsaturated zone is an important medium for the pollution of groundwater [Wang Donghai et al. 2000]. The contaminated unsaturated zone would pollute the groundwater under the infiltration of the atmospheric precipitation or irrigation. So in the human pursuit of economic development, we should pay more attention to the groundwater environment, strengthen the oil spill control pollutants, which is very important for the sustainable development of society and human health.

5 CONCLUSIONS

This paper mainly introduced the FVM for solving the three phase percolation model of unsaturated-saturated zone. In numerical terms, we used the circumcenter dual subdivisions which have better physical properties. And verify the method validity by way of example. Due to the FVM in the space satisfy the law of conservation of mass, however doesn't meet the law in the time, so time need to be controlled to ensure the stability of the calculation. In some parts of the known saturation unchanged, these points can be simplified in the calculation, to reduce the amount of computation and shorten the calculation time. Because the constitutive relationship is complex, it is need to simplify, otherwise, the circumcenter dual subdivisions require certain triangular nature, so they have a certain influence in the accuracy of the algorithm. In future work, we are hoping to combine the rational use of the constitutive relation to improve the accuracy of the algorithm. PREFERENCES, SYMBOLS AND UNITS

Consistency of style is very important. Note the spacing, punctuation and caps in all the examples below.

REFERENCES