Smoothed particle hydrodynamics method for numerical solution of multidimensional filtering problems

V Bashurov\textsuperscript{1} and V Zhigalov\textsuperscript{1}

\textsuperscript{1}Russian Federal Nuclear Center, Muzrukov ave., 10, Sarov, 607188, Russia

E-mail: bashurov@mail.ru, vlzhigalov@mail.ru

Abstract. The paper is devoted to solving the filtering problem for a mixture of water, gas, and oil in a homogeneous porous medium. The basic equations of filtration theory are converted into a special form for the numerical approximation with the smoothed particle hydrodynamics (SPH) method. A numerical difference scheme is constructed on the basis of SPH method. An algorithm for setting the boundary conditions is proposed and a number of isothermal 1D and 2D tests on the filtering process simulation for a mixture of water, oil, and gas.

1. Basic equations of filtration theory for mixtures in a porous medium

The problem of numerically simulating the dynamics of a multicomponent medium based on paper [1] is considered. It is assumed that the continuous medium is a system of pores, fractures, and faults, which typical dimensions are small in comparison with the physical size of the problem. The ratio of the pore volume to the total volume is the medium porosity metric:

$$m = V_p/V$$

where $m$ is the porosity coefficient, $V_p$ is the pore volume, $V$ is the total volume of a given element of the medium. The multicomponent mixture flow in porous media is called “filtration”. Here, a “component” is a part of the mixture with its own physical and chemical properties and with no changes in its phase state during the simulation. The main parameters of a moving system are the pressure, temperature, and saturation of each component. Saturation $S_k$ of the $k$-th component void space is the pore volume fraction occupied by this component in a volume element:

$$S_k = \frac{\Delta V_k}{\Delta V_p} k = 1,2\ldots n$$

where $n$ is the number of components in mixture. The summarised saturation of all components in a volume element equals 1:

$$\sum_{k=1}^{n} S_k = 1.$$  \hspace{1cm} (1)

There is a saturation minimum for each component. These values are called “residual saturations” (subscript $r$). The simultaneous flow of components takes place in a certain range of saturation values only. For the operation in this range of saturation values, the notion of effective saturations of the components
is introduced (effective saturations are denoted by the “upper bar” symbol). The effective saturation of the $k$-th component may be represented as:

$$\bar{S}_k = \frac{S_k - S_k^r}{1 - \sum_{i=1}^{n} S_i^r}.$$  

The basic filtration law (Darcy rule) establishes a relationship between the flow velocity vector and the pressure drop that causes the filtration flow. The flow velocity, $u_k$ for each component is written (regardless of the gravity force) in the following form:

$$u_k = -K \frac{c_k}{\mu_k} \nabla P_k$$  \hspace{1cm} (2)

where $K$ is the porous medium characteristic called “absolute permeability”, which is independent of the mixture properties; $\mu_k = \mu_k(T)$ is the dynamic viscosity coefficient of the $k$-th component; $c_k = c_k(S_n)$ is the relative phase permeability of the $k$-th component (it may depend on the saturation of other components); $P_k$ is the $k$-th component pressure. Another fundamental relationship in filtration theory is the mass conservation law. For each component it takes the form:

$$\frac{\partial (m \rho_k S_k)}{\partial t} + \text{div}(\rho_k u_k) = 0$$  \hspace{1cm} (3)

where $\rho_k$ is the $k$-th component density. Substitute (2) into expression (3) and obtain the main equation of filtration theory:

$$\frac{\partial (m \rho_k S_k)}{\partial t} = \nabla (\rho_k K \frac{c_k}{\mu_k} \nabla P_k).$$  \hspace{1cm} (4)

Equation (4) will be further used for approximation by the SPH method.

2. Equations of state for liquid and gas

The paper poses the problem of simulating a three-component mixture of gas, water, and oil with regard to their compressibility. For convenience, the following index notations are further used for these components: $w$ for water, $n$ for light oil (naphtha), and $g$ for gas. The initial values of saturation, temperature, and pressure are specified for each component. Densities are calculated from the corresponding equations of state of the components depending on the pressure and temperature. The water and oil components are considered to be weakly compressible and linearly dependent on the temperature and pressure gradients:

$$\rho_k = \rho_{0k} \left( 1 + \beta_k (P_k - P_0) + \alpha_k (T_k - T_0) \right)$$  \hspace{1cm} (5)

where $k = w, n$, and $\rho_{0k}$ is the known density value of the $k$-th component, corresponding to pressure $P_0$ and temperature $T_0$. As for gas, the equation of state of an ideal gas is assumed to be valid:

$$\rho_g = \rho_{0g} \frac{P_g T_0}{P_0 T_g}$$  \hspace{1cm} (6)

In the simulation the physicochemical parameters of the mixture, such as relative phase permeabilities and dynamic viscosities of the components are used. Thus, equations (4), (5), and (6) form a closed system which is solved with respect to pressures, densities, and saturations of the components.

3. Equation approximation with SPH method

The smoothed particle hydrodynamics (SPH) method [2] is based on smoothed integral interpolation of any scalar, or vector quantity specified in space. Smoothed interpolation $A_{SPH}(r)$ of some scalar quantity $A(r)$ is expressed as an integral:
\[ A_{SPH}(r) = \int_{-\infty}^{\infty} A(r') W(r - r', h) dr' \]  

(7)

where \( W(r - r', h) \) is an even function also called an “interpolation kernel”. Figure 1 graphically represents function \( W(r, h) \) (solid line) and its derivative, \( W'(r, h) \) (dashed line). The computational domain in the problem is partitioned into \( N \) elements with coordinates \( r_i \), where \( i = 1, N \). Each element is hereinafter referred to as a smoothed particle. Passing from integration to summation in (7) and replacing volume element \( dr' \) by the volume of smoothed particle, \( V_j \) we obtain the basic formula for the difference approximation of an arbitrary function \( A(r_i) \) in a given point \( r_i \):

\[ A(r_i) = \sum_{j=1}^{N} V_j A(r_j) W(r_i - r_j, h) \]  

(8)

Accordingly, the derivative of function \( A(r_i) \) with respect to \( r_i \) has the following form:

\[ \nabla A(r_i) = \sum_{j=1}^{N} V_j A(r_j) \nabla W(r_i - r_j, h) \]  

(9)

Equations (8) and (9) are the fundamental equations in SPH method. The right-hand side of equation (4) should be transformed for the subsequent approximation with SPH method. With \( \phi = -K \frac{c}{\mu} \) the right-hand side of equation (4) is identically transformed:

\[ \nabla (\phi \nabla A) = \frac{1}{2} (\nabla^2 (\phi A) - A \nabla^2 \phi + \phi \nabla^2 A) \]  

(10)

The right-hand side of equation (10) contains the sum of three Laplace differential operators which should be approximated with SPH method.

Figure 1. Smoothing function \( W \) (solid line) and its derivative \( W' \).

For the numerical approximation of Laplace operator, scalar quantity \( A(r) \) is expanded into Taylor series at neighboring points \( r_i \) and \( r_j \) in space:
A(r_j) - A(r_i) = \nabla A(r_i)(r_j - r_i) + \frac{1}{2} \nabla^2 A(r_i)(r_j - r_i)^2 + \frac{1}{6} \nabla^3 A(r_i)(r_j - r_i)^3 + O(r_j - r_i)^4

Upon truncation of the fourth-order and higher-order terms the both parts of the equation are multiplied by expression
\[
\frac{(r_j - r_i) \cdot \nabla W(r_j - r_i, h)}{|r_j - r_i|^2}
\]

Then, take \(r_{ij} = r_j - r_i\) and \(W_{ij} = W(r_j - r_i, h)\), integrate with respect to \(r_j\), and obtain the integral representation of Laplace operator and passing from integration to summation in the last formula and replacing volume element \(d^3r_j\) by the smoothed particle volume, \(V_j\) we obtain the difference equation to approximate the integral representation of Laplace operator:
\[
\nabla^2 A_i = -2 \sum_{j=1}^{N} V_j \frac{A_{j-A_i} r_{ij} \nabla W_{ij}}{|r_{ij}|^2}
\]

Laplace operators in the right-hand side of identical equation (10) are replaced by expression (11). After several simple arithmetic simplifications this identical equation is transformed to obtain
\[
\nabla(\phi_i \nabla A_i) = \sum_{j=1}^{N} V_j \frac{(\phi_{i} + \phi_{j})(A_{j-A_i})}{|r_{ij}|^2} r_{ij} \nabla W_{ij}
\]

Accordingly, equation (4) takes the final difference form:
\[
\frac{\partial (\rho_k S_{ki})}{\partial t} = \frac{\kappa}{m} \sum_{j=1}^{N} V_j \frac{(\rho_{k_{i}^{c_{ki}}} + \rho_{k_{p_{k_{j}}}^{c_{kj}}} - P_{i})}{|r_{ij}|^2} r_{ij} \nabla W_{ij}
\]

4. Time integration
To calculate thermodynamic parameters, an explicit difference scheme is used in the next time step. Let the right-hand side of equation (4) be \(F_{ki}\) we obtain the following differential equation:
\[
\frac{\partial (\rho_k S_{ki})}{\partial t} = F_{ki}
\]

The first-order difference scheme for the calculation of values at the next time layer for equation (14) looks like
\[
\rho_{ki}^{n+1} S_{ki}^{n+1} = \rho_{ki}^n S_{ki}^n + \Delta t \cdot F_{ki}
\]

where the superscript \(n\) denotes the corresponding quantity value at the time layer \(t = t_n\). The time integration step, \(\Delta t\) is chosen basing on the difference scheme stability condition in solving the Laplace equation, \(\Delta t = ch^2\) with \(c < 1\). As a result, a system of seven equations (1), (5), (6), and (15) with respect to seven unknowns \(P_{ki}^{n+1}, \rho_{ki}^{n+1}, S_{ki}^{n+1}\) where \(k = [W, g, n]\) is solved for each smoothed particle in space \(r_i\). Due solving this system of seven equations at each point \(r_i\), new values of pressure, density, and saturation of the components are calculated at the next time layer \(t = t_{n+1}\). One can easily see that the system of seven equations (1), (5), (6), and (15) is reduced to solving a cubic equation for pressure \(P_{ki}^{n+1}\).
5. Test computations
The initial conditions for tests are taken from [3]. In all problems, the rock porosity, density, and absolute permeability are considered invariable in the whole volume, the residual saturation values are assumed to equal zero, the computational domain size is $1 \times 1 \times 1$ m. One-dimensional and two-dimensional problems are solved in Cartesian coordinates. The mixture consists of gas, water, and light oil. For each component, the initial values of all dynamic parameters – saturation, temperature, and pressure - are considered to be specified.

| Table 1. The values of parameters for equations of state (5), (6). |
|------------------|------------------|------------------|
| $\rho_0$, kg/m$^3$ | $\beta$, 1/Pa $\times 10^{-7}$ | $\alpha$, 1/K $\times 10^{-7}$ |
| Water            | 1000             | 4.4              | 1.32             |
| Oil              | 850              | 10.0             | 9.2              |
| Gas              | 1.4              | -                | -                |

The medium is isotropic in the simulated volume. It is assumed that liquid phases are weakly compressible, gas is ideal, the temperature and pressure are the same for all mixture components. The temperature is considered invariable in the course of simulations. There is no gravity.

5.1. One-dimensional test on the gas injection under pressure
Figure 2 graphically represents computation results for a 1D test from paper [3]. These computations were carried out using an explicit difference scheme on a regular and space-uniform computational grid of 50 nodes.

\[\text{Figure 2. Saturation profiles from paper [3] at times } t = 5000\text{s (left) and } t = 25000\text{s (right)}\]

A one-dimensional test problem of an isothermal three-component flow is considered. A three-component mixture flows due to the difference in pressures at the ends of the segment under consideration in horizontal direction. The domain size is 1 m. Gas is injected under pressure from left to right. Initial conditions are $S_w = 0.4, S_n = 0.3, S_g = 0.3, P_w = P_{ATM}, T = 285K$. Boundary conditions for saturation and pressure: $S_g|_{x=0} = 0.7, S_w|_{x=0} = 0.15, S_n|_{x=0} = 0.15, P_w|_{x=0} = 1.1 \times P_{ATM}, P_w|_{x=1} = P_{ATM}$. The rock parameters used for calculations are, as follows: $K = 6.64 \times 10^{-11}$ m$^2$, $m = 0.4$. All constant values are given in the International System of Units (SI system). Testing is performed by varying the number of smoothed particles $N$ (from 10 to 20), the size of interpolation kernel $h$ (from 1.5 to 3.0 typical sizes of particles), and the method used to solve equations (1), (5), (6).
Results of computations with \( N=12 \) and \( h = 0.15 \text{m} \) are illustrated by figure 3 in the form of the saturation profiles of the components at time moments.

Figure 3. SPH simulation. Saturation profiles at times \( t = 5000 \text{s} \) (left) and \( t = 25000 \text{s} \) (right).

The results obtained are visually the same as those in paper [3].

5.2. Two-dimensional test on the gas injection under pressure

The physicochemical parameters and initial conditions for the computational domain in the two-dimensional test are the same as in the one-dimensional test described above. The computational domain size is \( 1 \text{ m} \times 1 \text{ m} \). Gas is injected from the left lower angle of the computational domain. The boundary values of saturation and pressure are \( S_g|_{x=0y=0} = 0.7 \), \( S_w|_{x=0y=0} = 0.15 \), \( S_n|_{x=0y=0} = 0.15 \), \( P_w|_{x=0y=0} = 1.1 \times P_{ATM} \), \( P_w|_{x=1y=1} = P_{ATM} \). Figure 4 shows the test results of SPH simulation at time \( t=5000 \text{ s} \) with the number of particles \( N = 11 \times 11 \) and uniform smoothing size \( h = 0.15 \text{m} \).

Figure 4. Pressure profile (left) and the saturations (right) of water (grid) and gas(solid surface) profiles at time \( t = 5000 \text{s} \).

6. Conclusion

In the numerical simulation of a real physical flow process (for example, oil production in an underground oil field) it is important to construct a three-dimensional computational grid in which the cell size in the oil well vicinity equals the typical size of the wellhead diameter (15-30 cm) and the cell size
on the oil field boundary is 10 to 50 meters. The smoothed particle hydrodynamics (SPH) method solves this problem. The research efforts resulted in the development and verification of SPH method to solve filtering problems, a prototype software package has been developed to simulate multidimensional filtering problems. The authors extends appreciation to Prof. S. P. Bautin for the discussion of the mathematical problem formulation, valuable advices, and assistance in writing the paper.

**Acknowledgments**

We would like to express our special thanks of gratitude to professor Sergey Bautin.

**References**

[1] Parker J, Lenhard R and Kuppusami T 1987 A parametric model for constitutive properties governing multiphase flow in porous media *Water Resources Research* **23** 618–624

[2] Gingold R and Monaghan J 1977 Smoothed particle hydrodynamics: theory and application to non-spherical stars *Mon. Not. Roy. Astron. Soc.* **181** 375-389

[3] Lyupa A, Trapeznikova M and Churbanova N 2016 Simulation of a non-isothermal multiphase flow using explicit difference schemes *IAM preprints* **103**