EDN: XYDYVJ
УДК 519.67

Verification of a Numerical Method for Modeling Two-phase Flows of Immiscible Liquids with the Transfer of Modifying Additives in Three-dimensional Digital Core Models

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Received 10.08.2024, received in revised form 17.09.2024, accepted 27.10.2024

Abstract. This paper presents the results of development and testing of the calculation method and software for modeling two-phase immiscible flows in three-dimensional digital core models taking into account the transfer of modifying additives (surfactant/polymer solutions and nanosuspensions) during flooding. The mathematical model is based on the Navier–Stokes equations and the VOF cell fluid method. The developed numerical method was tested on the problem of two-phase filtration during oil displacement in a three-dimensional model of a porous medium. Cross-verification with the Ansys Fluent CFD software package was performed. As a result of testing and cross-verification, it was shown that the numerical solutions obtained using the developed numerical method and software are in good qualitative and quantitative agreement with the numerical solutions obtained using Ansys Fluent. At the same time, a more than threefold gain in calculation speed was demonstrated compared to the Ansys Fluent software package.

Keywords: digital core models, immiscible displacement, VOF method, testing.

Citation: A.A. Gavrilov, D.V. Guzei, A.A. Dekterev, A.V. Minakov, Verification of a Numerical Method for Modeling Two-phase Flows of Immiscible Liquids with the Transfer of Modifying Additives in Three-dimensional Digital Core Models, J. Sib. Fed. Univ. Math. Phys., 2024, 17(6), 817–828. EDN: XYDYVJ.

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Introduction

Currently, digital technologies are being developed, with one area of focus being digital core models. This technology enables the acquisition of supplementary data regarding rock samples through the numerical simulation of physical processes, complementing traditional laboratory studies. The standard methods for estimating the formation parameters, such as geophysical and hydrodynamic well testing, as well as laboratory core studies have a number of disadvantages. Among these, we note the complexity and sometimes impossibility to obtain and process quality core material in sufficient quantities; high cost and practical impossibility of mass application of a number of methods of laboratory studies; impossibility to conduct multiple experiments on a single sample, and, as a consequence, non-reproducibility, in the strict sense, of research results; impossibility to recreate the full range of reservoir conditions and to conduct full-fledged parametric studies [1–4]. At the same time, the advancement of innovative techniques for oil recovery enhancement necessitates a comprehensive investigation of the prevailing patterns of physical and chemical processes during multiphase filtration in porous media. The utilization of digital core models facilitates the undertaking of systematic studies of novel methods of enhanced oil recovery.

The digital core approach is an integrated methodology that aims to obtain the volumetric topology of rock pore space and its physical and chemical properties. This is achieved through the utilization of computer tomography techniques and subsequent application of computer simulation methods for multiphase flows, which are employed to investigate the reservoir porosity and permeability.

In the long term, digital core models are regarded as a potential substitute for conventional filtration experiments utilizing authentic core samples. Numerical simulations of flows in digital cores are conducted using a variety of methods. One of the most frequently employed methods for numerical simulation of two-phase flows is the direct numerical simulation (DNS) approach with the interfacial front tracking [6–9]. In this approach, the most commonly employed techniques are based on the VOF method [6], the level-set function method (LSM) [7], and a variety of the phase-field models [8]. Each of these methods possesses distinctive advantages and disadvantages, and exhibits notable differences in terms of its performance, versatility, and the reliability of the numerical algorithm. Moreover, various variants of the lattice Boltzmann equation method (LBM) have recently been employed with great success in the study of two-phase flows in numerical core models [9].

Despite the fact that the direction of application of numerical modeling for the study of multiphase flows in digital core models is currently developing intensively, there are still many unresolved issues related to increasing the productivity and reliability of the calculation algorithms and software developed for this purpose. This paper presents the intermediate results of the development and verification of a calculation technique for modeling two-phase immiscible flows in three-dimensional digital core models taking into account the transfer of modifying additives (surfactants, polymers and nanoparticles) during flooding.

1. Mathematical model of two-phase immiscible flow in digital core models

Based on the program core of the domestic CFD SigmaFlow program complex [10–12], a numerical method for describing the unsteady flow process of immiscible fluids in three-dimensional digital core models with phase interface resolution was developed based on the Navier–Stokes

model for incompressible fluid and the VOF method [13] taking into account surface tension forces and surface wetting effects, also implemented the effect of the transfer of modifying additives (surfactant/polymer solutions and nanosuspensions) during the flooding process. The displacing fluid (index 1) is supplied at the inlet to the computational domain, while the displaced fluid (index 2) fills the computational domain at the initial moment of time. The two-phase medium is treated as a single-fluid medium consisting of two components and having a continuous density and viscosity distribution:

$$\rho = \alpha\rho_1 + (1-\alpha)\rho_2; \quad \mu = \alpha\mu_1 + (1-\alpha)\mu_2. \tag{1}$$

The fluid flow is described by the Navier–Stokes equations for an incompressible medium:

$$\bigtriangledown \cdot \mathbf{u} = 0 \tag{2}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\bigtriangledown)\mathbf{u}\right) = -\bigtriangledown p + \bigtriangledown\cdot(2\mu\mathbf{S}) + (\rho-\rho_\infty)\mathbf{g} + (\mathbf{f}_c - \bigtriangledown p_c) \tag{3}$$

where $\mathbf{u}$ is the velocity vector, p is the dynamic pressure, is the strain rate tensor, $\mathbf{S} = 0.5(\bigtriangledown\mathbf{u} + \bigtriangledown\mathbf{u}^T)$ is the characteristic density, $\mathbf{f}_c$ is the bulk surface tension force, and p_c is the capillary pressure.

The fluids are assumed to be immiscible with a well-defined interface.A modifying additive with a mass concentration of ϕ may be present inside the aqueous phase. The transfer equation for the fluid interface marker, or volume fraction of liquid 1, or indicator function is of the form:

$$\frac{\partial\alpha}{\partial t} + \bigtriangledown\cdot(\mathbf{u}\alpha) = 0 \tag{4}$$

The capillary pressure is extracted from the total pressure and is described by the equation:

$$\bigtriangledown\cdot\bigtriangledown p_c = \bigtriangledown\cdot\mathbf{f}_c, \tag{5}$$

with Neumann-type boundary conditions at the interfaces. The surface tension force ($\mathbf{f}_c$) if simulated by a volume force according to the CSF (continuum surface force) model [14].

In digital core problems, it is important to be able to calculate the efficiency of oil recovery enhancement methods. The most common methods include chemical methods, such as flooding with polymers and surfactants, including nanosuspensions. To model the transfer of modifying additives during secondary flooding, a mathematical model was developed and a software module was implemented. Polymer solutions, surfactants or nanomaterials can act as modifying additives. Within the framework of this approach, a convective-diffusion mechanism for the transfer of a modifying additive within only the aqueous phase is implemented, taking into account the influence of the local concentration of the additive on viscosity, interfacial tension and contact angle.

The equation for the transfer of modifying additive concentration ϕ in the carrier phase α is written as:

$$\frac{\partial(\alpha\phi)}{\partial t} + \bigtriangledown\cdot(\mathbf{u}\alpha\phi) - \bigtriangledown\cdot(\alpha D_\phi \bigtriangledown\phi) = 0, \tag{6}$$

where D_ϕ — diffusion coefficient of structural elements of the impurity [m^2/s].

A Dirichlet-type boundary condition is set at the inlet boundary. A Neumann-type boundary condition is set on the solid walls and the outlet boundary. The presence of an impurity in the volume leads to a change in the properties of the mixture (impurity and carrier phase) and the conditions at the phase boundary. In the current version of the model, the change in the

properties of A (viscosity coefficient, interfacial tension and contact angle) is specified by a power formula depending on the concentration of the modifying additive ϕ:

$$A(\phi) = A_0(1 + c_1\phi + c_2\phi), \tag{7}$$

where A_0 — value of the property without impurity, c_1 and c_2 — model coefficients determined from experiments. In the current version, three properties are modeled: the viscosity of the carrier fluid, the surface tension coefficient, and the contact angle.

The numerical implementation is based on a modified transfer equation:

$$\frac{\partial(\phi)}{\partial t} + \bigtriangledown \cdot (\mathbf{u}\phi + (1-\alpha)\mathbf{u}_r\phi) - \bigtriangledown \cdot (\alpha D_\phi \bigtriangledown \phi) = 0. \tag{8}$$

The discretization of the impurity transport equation is constructed similarly to the transport equation of the indicator function with the inclusion of a diffusion term:

$$V_p\left(\frac{\partial\phi}{\partial t}\right) + \sum_f \phi_f \left[(\mathbf{u}_f + (1-\alpha)_f\mathbf{u}_r)\cdot\mathbf{S}_f\right] - \sum_f (D_\phi\alpha)_f (\bigtriangledown\phi_f \cdot \mathbf{S}_f) = 0. \tag{9}$$

The numerical method is based upon a technique [15] developed expressly for the resolution of displacement problems. The principal elements of the algorithm are outlined below. The numerical algorithm is based on the finite volume method for an unstructured mesh [16]. To obtain the balance relations of the finite volume method, integration of the differential equations over the volume of the mesh cell is performed with the volume integrals reduced to integrals over the surface of the reference volume. In order to mitigate the spatial smoothing of the interface in the numerical solution of the phase fraction transfer equation, the antidiffusion method is employed. The unsteady terms of the transport equations are approximated with an implicit first-order approximation. To approximate the convective terms of the Navier–Stokes equations and the transport equation of the modifying additive, the UMIST TVD scheme is used. The solution of the original system of equations is conducted sequentially. At each time step, several global iterations are performed to relate the velocity, pressure, and phase fraction fields. The loop of global iterations starts with the solution of the interface transport equation. The systems of difference equations, approximating the transport equations, are solved by the incomplete LU factorization iterative method. Systems of linear equations resulting from discretization of the elliptic equations for pressure correction and capillary pressure are solved using the algebraic multigrid method.

Boundary conditions. At solid walls, the velocity satisfies the no-flow and no-slip conditions, while the normal derivative of pressure is set to zero. At the inlet interface, the velocity and phase fraction are set constant. At the outlet interface, the flow homogeneity condition is set, which is expressed in the equality of zero normal derivatives of all scalar quantities.

Time step. For unsteady calculation with capillary stress at the phase interface, the time step is chosen from the condition [17] and is additionally limited by the convective Courant number (or CFL) at the phase interface, which by default does not exceed 0.1.

2. Testing results of the numerical method

The software product, being developed for calculation of two-phase flow during oil displacement from a porous medium, was subjected to testing. The calculation technique was based

on the solution of the Navier–Stokes equations, employing the VOF method, and taking into account the interfacial tension and the wetting effects of rock walls by fluids. The calculations were conducted using a three-dimensional model of a porous medium, which was constructed using a set of cylinders of varying diameters. The geometry of the computational domain was that of a rectangular section of a parallelogram with a fractured medium. The dimensions of the computational domain were as follows: length, 0.6 mm; width, 0.2 mm; and depth, 0.042 mm. A computational mesh was constructed, comprising a total of 2,754,380 computational voxels. A portion of the computational mesh is illustrated in Fig. 1. It is important to note a significant feature of voxel models of computational meshes. Given that the mesh is constituted by homogeneous cubic cells, the computational domain boundary is represented by a broken surface rather than a smooth one. The use of coarse meshes in complex-shaped channels results in the generation of an additional error compared to the use of computational meshes, wherein the faces of the meshes are parallel to the boundaries of the computational domain.

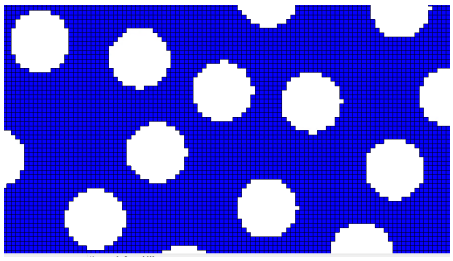


Fig. 1. Fragment of the computational grid

In this case, the direction of flow of the displacing medium along the X-axis. At the initial time point, the computational domain was filled with the model oil. Subsequently, water was introduced to the inlet of the computational domain, resulting in the displacement of the oil. The following physical properties of oil were employed in the calculation: density $\rho_2 = 800\ kg/m^3$ and dynamic viscosity $\mu_2 = 0.05\ Pa \times s$. The physical properties of water were: density $\rho_1 = 1000\ kg/m^3$ and dynamic viscosity $\mu_1 = 0.001\ Pa \times s$. The surface tension coefficient was $\sigma = 0.025\ N/m$. A constant velocity of $U = 2.5 \times 10^{-2}\ m/s$ was set at the inlet to the computational domain, which corresponds to the capillary number ($Ca = (\mu_1 U)/\sigma$) equal to 1×10^{-3}. A Neumann boundary condition was imposed at the outlet. The no-slip condition and the contact angle of 30 degrees were set at the walls of the computational domain.

The results of the computations were compared with those obtained using the Ansys Fluent software package. The Ansys Fluent software package was also utilized with a VOF-based two-phase solver, which employed geometric reconstruction of the phase interface and a continuum surface force procedure to calculate interfacial tension forces. Comparisons were made between the water and oil fraction dependences as a function of time, as well as between the pressure drop dependences as a function of time. Furthermore, the dependencies of fluid flow rate at the outlet from the computational domain were also compared. It is noteworthy that the calculations performed with both software products utilized the same voxel model. This allows for more rigorous verification of the developed software not only in terms of the main simulation results but also in terms of the time input required for computations. Fig. 2 illustrates the comparison of the phase distribution fields in the central section of the computational domain during the process of filling with water at analogous time points. The blue color indicates the oil, while the

red color indicates the water. A comparison of the phase distribution fields obtained by means of different software products has demonstrated that the outcomes of the process simulation of oil displacement by water are qualitatively satisfactory. Although the specific details of the phase interphase in both solvers vary, the general structure of the two-phase flow and the position of the displacement front at comparable time points generally agree. A distinctive feature of flow simulation in digital core models is the potential for significant variation in the dimensions of the pores and channels under consideration within a single computational domain. In this instance, a uniform computational mesh comprising cubic cells, or voxels, is employed for the computations. It is conceivable that there may be just two to three computational cells for each width of the flow channel. Such instances are not uncommon in models obtained through tomography of a real core. This necessitates more rigorous specifications for the calculation algorithm, particularly in the context of two-phase flow with a moving phase interface. For example, the issue of artificial blurring of the phase interface resulting from numerical diffusion in the numerical solution of the convective transport equation within the VOF method is a well-known problem. An analysis of the phase interface front in Fig. 2 indicates that both solvers are generally capable of addressing this issue. The blurring of the phase interface does not exceed two or three computational cells. Thus, the developed solver is comparable to the known Ansys Fluent software package.

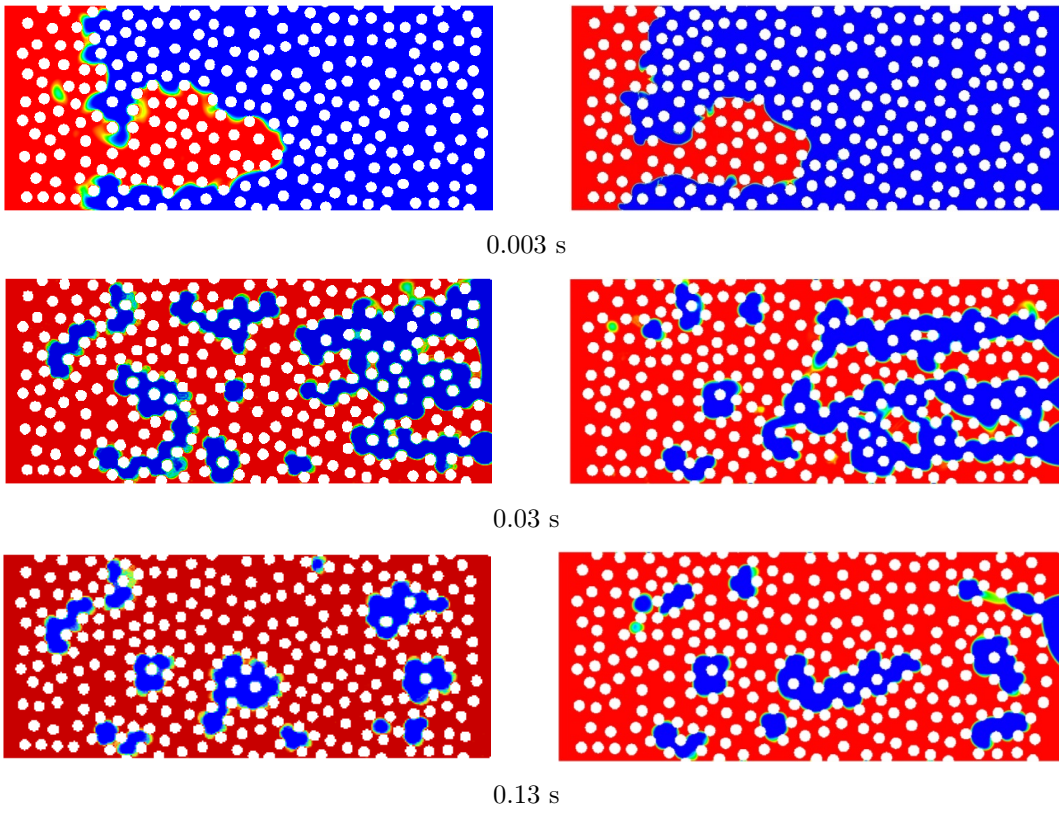
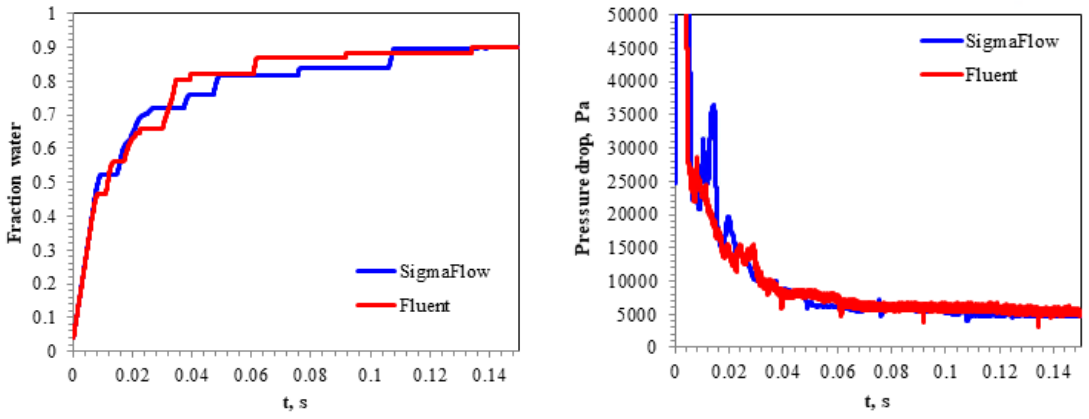


Fig. 2. Oil displacement dynamics by water (red): Ansys Fluent (left), SigmaFlow (right)

For each of the two phases, the time dependence of the liquid fraction was plotted. The liquid fraction was calculated as the ratio of the phase volume (V_i) at a given moment to the

total volume of pore space (V). According to the results of the computations performed with both the developed software and Ansys Fluent, the dependences of the phase fraction on time were plotted and compared. The dependence of the water volume fraction on time in the course of displacement is presented in Fig. 3(a). As can be seen, initially these dependences have a linear segment corresponding to pressure-driven displacement. In this mode, the displaced oil volume at the outlet is precisely equal to the volume of water entering at the inlet. This occurs until the water reaches the outlet from the computational domain. In the case under consideration, this occurs at approximately 0.008 second. Subsequently, the time dependence of the phase fraction exhibits a gradual stabilization, displaying a slightly slanting character throughout this period. The water continues to emerge in the form of discrete drops or larger plugs. As illustrated by the curves in Fig. 3(a), this phenomenon manifests as a sudden change in the behavior of the curve. The flow gradually reaches a state of complete stabilization, resulting in a zero oil flow rate at the outlet. The residual oil of approximately 10% is retained by capillary forces. As illustrated in Fig. 3(a), the results align well with those obtained by Ansys Fluent, with the maximum discrepancy in the time-dependent water phase fraction not exceeding 3%. At the conclusion of the displacement process (time point of 0.15 s in the plot), this discrepancy does not exceed 0.3%. Additionally, the time dependence of the pressure drop in the computational domain was plotted (see Fig. 3(b)). The pressure drop in the displacement process is also a crucial parameter, since it determines the relative phase permeability of the digital core model. The analysis demonstrates a satisfactory degree of concordance between the two solvers with respect to this parameter.



(a) (b)

Fig. 3. Dependence of the fraction of the displacing phase (a) and the pressure drop (b) on time

In addition to the accurate reproduction of reservoir porosity and permeability, another crucial requirement for digital core problems is the appropriate time expenditure. Modern three-dimensional tomography-derived digital core models can have a dimensionality of 1000^3 or even more voxels. Accordingly, the time invested in flow simulation in such systems can be considerable and pivotal for the subsequent utilization of this technology. The testing performed permitted an evaluation of the computational speed of the developed software product, which was compared with that of Ansys Fluent. The calculations were performed on a system with 32 cores and a core frequency of 4 GHz. The results of the comparison in terms of the machine

time consumed by both software packages to reach 0.08 s of physical time in the two-phase displacement process are presented in Tab. 1. The presented data demonstrate that the developed software exhibits 3.62 times increase in computational speed compared to that of Ansys Fluent. This is attributable to the more efficacious methodology employed for determining the adaptive time step in the developed solver.

Table 1. Comparison of time inputs of the considered solvers

	Estimated time, s	Real time, hh:min
SigmaFlow	0.08	21:54
Ansys Fluent	0.08	79:40

The developed model was tested to describe a multiphase flow in a model porous medium with surfactant/polymer/nanosuspension transport within the VOF model. In this paper, a model case was considered in which the additive to the displacing fluid affected only the viscosity coefficient (within the Newtonian model). Real polymer solutions were used as model solutions of displacing media in the calculations; their properties (dependences of the surface tension coefficient, contact angle and viscosity on concentration) were determined experimentally by us earlier [18]. The dependence for the viscosity coefficient was constructed based on experimental data for the polyacrylamide polymer Polyfloc A2020 in the concentration range from 0 to 0.1 wt.%. Calculations were performed on the displacement of the oil model from the model medium during the post-displacement process: first, pure liquid was pumped until the saturation level was established, and then an additive was fed to the inlet, which affected the properties of the displacing liquid. The moment of the start of the additive introduction on the graphs is shown by a vertical dotted line.

The following physical properties of oil were employed in the calculation: density $\rho_2 = 727.42$ kg/m^3 and dynamic viscosity $\mu_2 = 0.048$ Pa×s. The physical properties of water were: density $\rho_1 = 997$ kg/m^3 and dynamic viscosity $\mu_1 = 0.00102$ Pa×s. The surface tension coefficient was $\sigma = 0.0253$ N/m. A constant velocity $U = 3 \times 10^{-3}$ m/s was set at the inlet to the computational domain, which corresponds to the capillary number ($Ca = \mu_1 U/\sigma$) equal to 1.2×10^{-4}. A Neumann boundary condition was imposed at the outlet. The no-slip condition and the contact angle of 160 degrees were set at the walls of the computational domain. Fig. 4 and 5 show the phase distribution fields after displacement by water and the phase distribution fields and the polymer concentration in the steady-state filtration mode. Fig. 6 shows the graphs of the dependences of the proportion of the displacing fluid on time for two values of the concentration of the additive supplied at the entrance to the calculation area. The graphs also show the results of Ansys Fluent calculations for verification of the software product being developed. As can be seen from the presented dependencies, in the steady-state sections there is good agreement between the calculation results and the difference between SigmaFlow and Ansys Fluent does not exceed 1%.

Conclusions

1. A computational method and software have been developed to describe the flow of immiscible fluids with phase interface resolution based on the Navier–Stokes model and the VOF method in three-dimensional numerical core models, taking into account the transfer of modifying

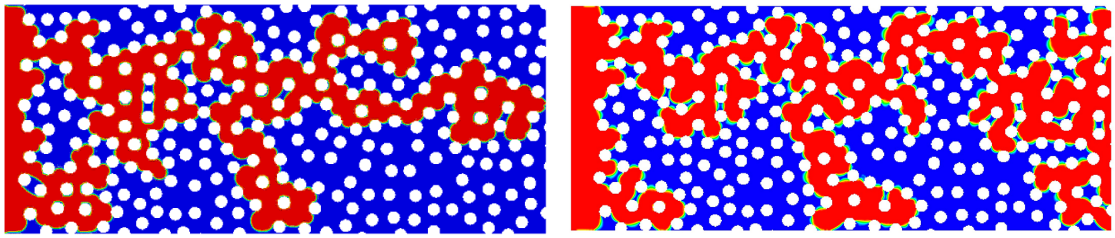
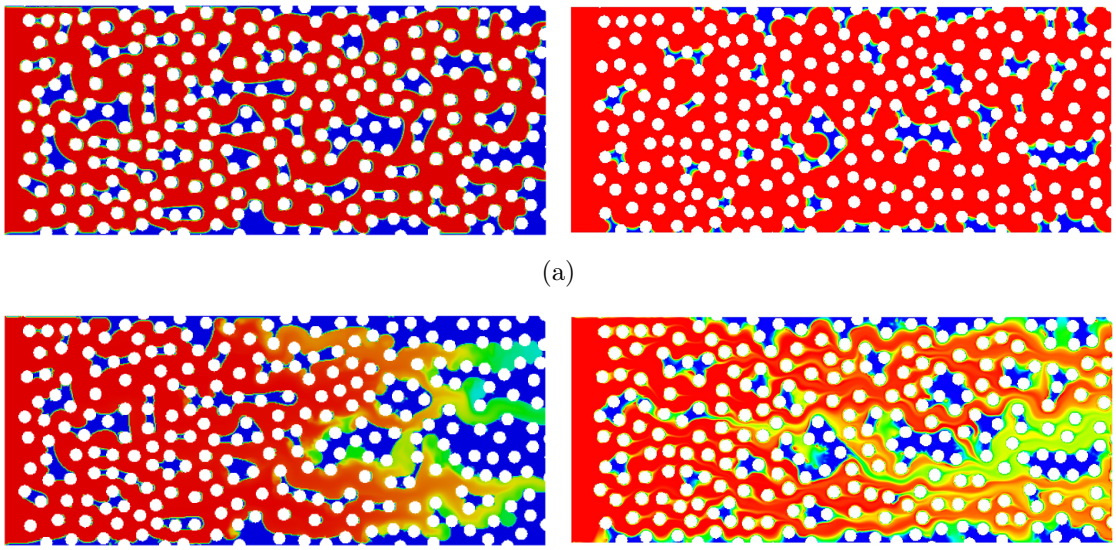


Fig. 4. Oil displacement dynamics by water (red): Ansys Fluent (left), SigmaFlow (right) (right)



(a)

(б)

Fig. 5. Distribution of phases (a) and polymer concentration (b) after displacement with water with an additive with an initial concentration of 0.1 wt.%: Ansys Fluent (left), SigmaFlow (right)

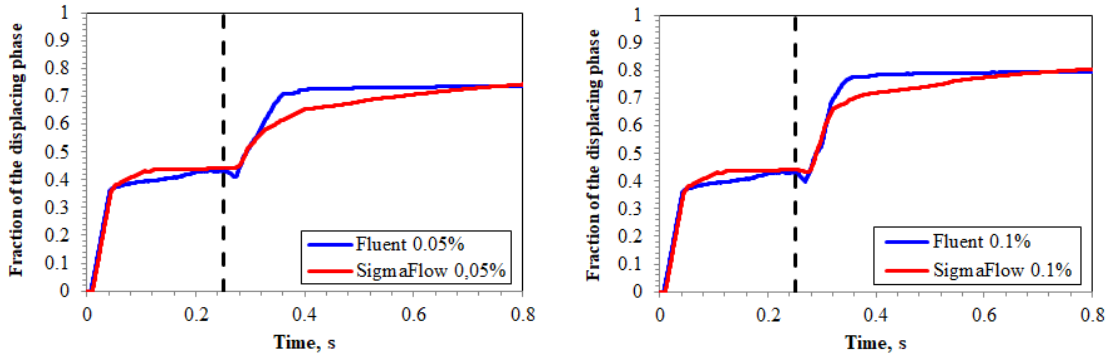


Fig. 6. Dependence of the fraction of the displacing phase on time for different concentrations of the additive at the inlet

additives (surfactant/polymer solutions and nanosuspensions) during flooding. The numerical algorithm is based on the control volume method for orthogonal and homogeneous voxel models of computational meshes. The peculiarity of the model is the separation of the capillary pressure component and hydrodynamic component from the total pressure. The equation describing capillary pressure component has the form of Poisson's equation. Surface tension is parameterized by bulk forces according to the continuum surface force (CSF) model. In order to mitigate the spatial smoothing of the phase interface that arises when numerically solving the transfer equation of the indicator function, the local antidiffusion method is employed. The time step is constrained by the characteristic capillary time on the scale of the spatial step and the condition of smallness of the Courant number at the phase interface. The time step is limited by the characteristic capillary time on the scale of the spatial step and the condition of smallness of the Courant number at the interface.

2. The developed numerical method was tested on model problems of two-phase filtration in a porous medium during oil displacement followed by additional oil displacement with a polymer solution. The developed numerical technique was evaluated through the tests conducted on a model problem of two-phase filtration during oil displacement in a three-dimensional model of a porous medium. Cross-verification was conducted using the Ansys Fluent CFD software package. Following a process of rigorous testing and cross-verification, it was demonstrated that the numerical solutions generated through the application of the developed numerical method and software exhibited a high degree of qualitative and quantitative agreement with those obtained using the previously known multiphase solver. Concurrently, the enhanced stability of the developed numerical algorithm against the emergence of parasitic vortex flows at the phase interface permitted 3.62 times increase in calculation speed, under identical conditions in comparison to that of Ansys Fluent.

This research was supported by the Russian Science Foundation grant no. 23-79-30022, https://rscf.ru/project/23-79-30022/.

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Верификация численной методики моделирования двухфазных потоков несмешивающихся жидкостей с переносом модифицирующих добавок в трехмерных цифровых моделях керна

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Аннотация. В статье представлены результаты разработки и тестирования расчетной методики и программного обеспечения для моделирования двухфазных несмешивающихся потоков в трехмерных цифровых моделях керна с учетом переноса модифицирующих добавок (растворы ПАВ/полимеров и наносуспензий) в процессе заводнения. Математическая модель основана на уравнениях Навье–Стокса и методе жидкости в ячейках VOF. Проведено тестирование разработанной численной методики на задаче двухфазной фильтрации при нефтевытеснении в трехмерной модели пористой среды. Выполнена кросс-верификация с пакетом программ Ansys Fluent. В результате тестирования и кросс-верификации было показано, что численные решения, полученные с помощью разрабатываемой численной методики и программного обеспечения качественно и количественно хорошо согласуются с численными решениями, получаемыми с помощью использования программ Ansys Fluent. При этом был продемонстрирован более чем трехкратный выигрыш в скорости расчета по сравнению с пакетом программ Ansys Fluent.

Ключевые слова: цифровые модели керна; несмешивающиеся вытеснения; VOF метод; тестирование.