

# **SIMULATION OF MULTIPHASE FLOWS IN POROUS MEDIA WITH THE FLUX RELAXATION**

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**Abstract.** The work deals with the development of explicit algorithms for the simulation of multiphase flow of slightly compressible fluid in the subsurface. Two approaches to deriving a hyperbolized system of equations are proposed and studied numerically. An original model is developed via the principle of minimal sizes and the differential approximation technique. Another model is obtained due to the introduction of the mass flux relaxation into the continuity equation. Approximations by three-level explicit difference schemes allow increasing the time step at least by an order of magnitude in comparison with two-level schemes for the classical model.

## **1 INTRODUCTION**

The development of robust computational technologies including adequate mathematical models, accurate numerical methods and efficient parallel codes to predict large-scale processes in the subsurface is one of urgent tasks of industrial mathematics. Among the possible applications there are optimisation of oil and gas recovery, solution of ecology problems concerning contaminant infiltration into the soil, construction of land reclamation and hydraulic facilities etc.

The major goal of the research is the creation of explicit algorithms for the simulation of multiphase compressible fluid flow in a porous medium. The interest in explicit schemes is explained by a number of valid reasons. Some problems (e.g., oil recovery with combustion fronts or phase transitions) require calculations with very small space steps constraining the time step strictly. Then explicit schemes can surpass implicit ones in terms of the total run time. Besides that explicit methods are preferable for adaptation to HPC systems.

An original approach to modeling porous medium flows [1] is developed by the authors in accordance to this trend. The model is derived by the analogy with the quasi-gas dynamic (QGD) system of equations [2] and modified to change the continuity equation type from parabolic to hyperbolic. Consequently an explicit scheme with a milder stability condition can be used for the approximation.

The present paper reports another approach to deriving hyperbolized equations. Currently the description of physical phenomena in consideration of the time of propagation of perturbations and the time of alignment of macroparameters (e.g., the pressure, the temperature, the density) becomes increasingly widespread [3]. In order to account for this time it is proposed to introduce the mass flux relaxation into the continuity equation. This technique is applied to the simulation of compressible fluid flow in a porous medium for the first time. Test predictions show advantages of the both approaches, in particular, the accuracy and the possibility to decrease the time step restriction at computations via explicit difference schemes.

## 2 THE CLASSICAL MODEL OF FLUID FLOW IN A POROUS MEDIUM

The governing model for isothermal multiphase fluid flow in a porous medium can be written as follows (the subscript  $\alpha = w, n, g$  denotes the phase –water (w), Non-Aqueous Phase Liquid (n), gas (g)) [4, 5]:

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \operatorname{div} \rho_\alpha \mathbf{u}_\alpha = q_\alpha \quad (1)$$

$$\mathbf{u}_\alpha = -K \frac{k_\alpha(S_w)}{\mu_\alpha} (\operatorname{grad} P_\alpha - \rho_\alpha \mathbf{g}) \quad (2)$$

$$\rho_\alpha = \rho_\alpha(P_\alpha) \quad (3)$$

$$\sum_\alpha S_\alpha = 1 \quad (4)$$

Here  $S_\alpha$  is the saturation,  $P_\alpha$  is the pressure,  $\rho_\alpha$  is the density,  $\mathbf{u}_\alpha$  is the Darcy velocity,  $\phi$  is the porosity,  $K$  is the absolute permeability,  $k_\alpha(S_w)$  is the relative phase permeability,  $\mu_\alpha$  is the dynamic viscosity,  $q_\alpha$  is the source of fluid,  $\mathbf{g}$  is the gravity vector. The above system consists of the continuity equation (1), the generalized Darcy law (2), the state equation (3) and the closing relation (4). The next assumptions are used: the porous medium is non-deformable and isotropic, fluids are immiscible, non-interacting and do not dissolve, phase transitions are absent, liquids are slightly compressible, gas is ideal, capillary forces are taken into account.

The current research focuses on two-phase cases: water/air and water/oil flows are discussed. System (1)-(4) is completed by constitutive relationships for the relative phase permeabilities and the pressure difference between phases (the capillary pressure) as a function of saturation. They are represented by the van Genuchten model [5] formulated in terms of the effective saturation of water ( $S_{we}$ ):

$$k_w(S_{we}) = S_{we}^{\frac{1}{2}} \left[ 1 - \left( 1 - S_{we}^{\frac{N}{N-1}} \right)^{\frac{N-1}{N}} \right]^2 \quad (5)$$

$$k_g(S_{we}) = \left( 1 - S_{we} \right)^{\frac{1}{2}} \left[ 1 - S_{we}^{\frac{N}{N-1}} \right]^{\frac{2(N-1)}{N}}$$

$$P_g - P_w = P_{c\,gw}(S_{we}) = \frac{1}{\alpha} \left[ \left( S_{we} \right)^{\frac{N}{1-N}} - 1 \right]^{\frac{1}{N}} \quad (6)$$

$$S_{we} = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}}. \quad (7)$$

where  $S_{wr}$  and  $S_{nr}$  are residual saturations of water and NAPL correspondently,  $\alpha$  and  $N$  are some parameters.

### 3 THE KINETIC APPROACH TO POROUS MEDIUM FLOW SIMULATION

#### 3.1 QGD-based model and computational algorithm

Among modern methods of computational fluid dynamics kinetic algorithms such as the Lattice Boltzmann schemes and the kinetically consistent finite difference (KCFD) schemes [2] are very popular. The derivation of KCFD schemes and the related QGD system of equations is based on the so-called principle of minimum sizes. This principle states the fact that in the numerical solution of a number of problems of continuum mechanics it makes no sense to consider scales smaller than some minimal reference length. In porous media this length  $l$  is a distance at which rock microstructure is negligible ( $l$  is of the order of hundred rock grain sizes). The minimal reference time  $\tau$  is assumed to be the time for inner equilibrium establishing in the volume of linear size  $l$ . Starting from the basic equation (1), using the principle of minimal sizes and the differential approximation technique the next modified phase continuity equation has been derived [1]:

$$\phi \frac{\partial(\rho_\alpha S_\alpha)}{\partial t} + \tau \frac{\partial^2(\rho_\alpha S_\alpha)}{\partial t^2} + \text{div}(\rho_\alpha \mathbf{u}_\alpha) = q_\alpha + \text{div} \frac{l c_\alpha}{2} \text{grad}(\rho_\alpha S_\alpha) \quad (8)$$

Here  $c_\alpha$  is the sound speed in  $\alpha$ -phase.

Equation (8) has a regularizing term and a second order time derivative with small parameters. The regularizer allows using central differences for the convective term approximation, the hyperbolic type of the equation leads to a three-level explicit scheme with a milder stability condition in comparison with explicit schemes for the parabolic equation (1).

It is proposed to use linear state equations for slightly compressible liquids and the ideal gas state equation if the gas phase is accounted for in calculations:

$$\rho_\alpha = \rho_{0\alpha} [1 + \beta_\alpha (P_\alpha - P_{0\alpha})], \quad \alpha = w, n \quad (9)$$

$$\rho_g = \rho_{0g} \frac{P_g}{P_{0g}} \quad (10)$$

Here  $\beta_\alpha$  is the coefficient of isothermal compressibility,  $P_{0\alpha}$  and  $\rho_{0\alpha}$  are reference values.

A computational algorithm of the explicit type has been developed for numerical implementation of the modified model (8), (2), (9)-(10), (4)-(7). In case of two-phase water/gas flow when  $P_g$  and  $S_w$  are chosen as primary variables the algorithm is described below.

Starting from the initial and boundary conditions for  $P_g$  and  $S_w$  on each  $j$ -th time level ( $j = 1, 2, \dots$ ) the next sequence of operations are fulfilled:

- Computation of  $S_g^j$  from (4),  $k_\alpha^j = k_\alpha(S_w^j)$ ,  $P_{c_{gw}}(S_w^j)$  and then  $P_w^j$  from (5)-(7);
- Computation of phase densities  $\rho_\alpha^j$  from (9), (10);
- Computation of Darcy velocities  $\mathbf{u}_\alpha^j$  from (2);
- Computation of the term  $(\rho_\alpha S_\alpha)^{j+1}$  from (8) for the both phases via a three-level explicit scheme;
- Computation of  $P_g^{j+1}, S_w^{j+1}$  solving the following system of nonlinear algebraic equations locally at each point of the grid (the system is formed by state equations multiplied by unknowns  $S_\alpha^{j+1}$ , there are the just found values  $(\rho_\alpha S_\alpha)^{j+1}$  in the right-hand sides)

$$\begin{aligned} \rho_{0w} \left[ 1 + \beta_w (P_g^{j+1} - P_{c_{gw}}(S_w^{j+1}) - P_{0w}) \right] S_w^{j+1} &= (\rho_w S_w)^{j+1} \\ \rho_{0g} P_g^{j+1} / P_{0g} (1 - S_w^{j+1}) &= (\rho_g S_g)^{j+1} \end{aligned} \quad (11)$$

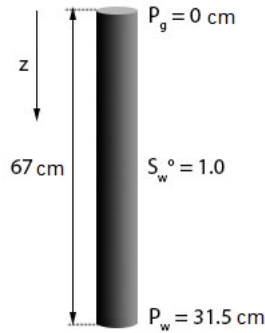
This system can be solved, for example, by Newton's method that takes only a few iterations.

- Data exchange at multiprocessor computing.

The presented model and algorithm are generalized successfully to the case of three-phase fluid flow, high parallelization efficiencies are achieved at computations on hybrid supercomputers [1].

### 3.2 Drainage test problem

For verification of the above model and algorithm it is proposed to solve numerically a drainage test problem carefully studied in [5]. The process of two-phase (water/air) isothermal infiltration due to the gravity is simulated. The geometry is illustrated by Figure 1.

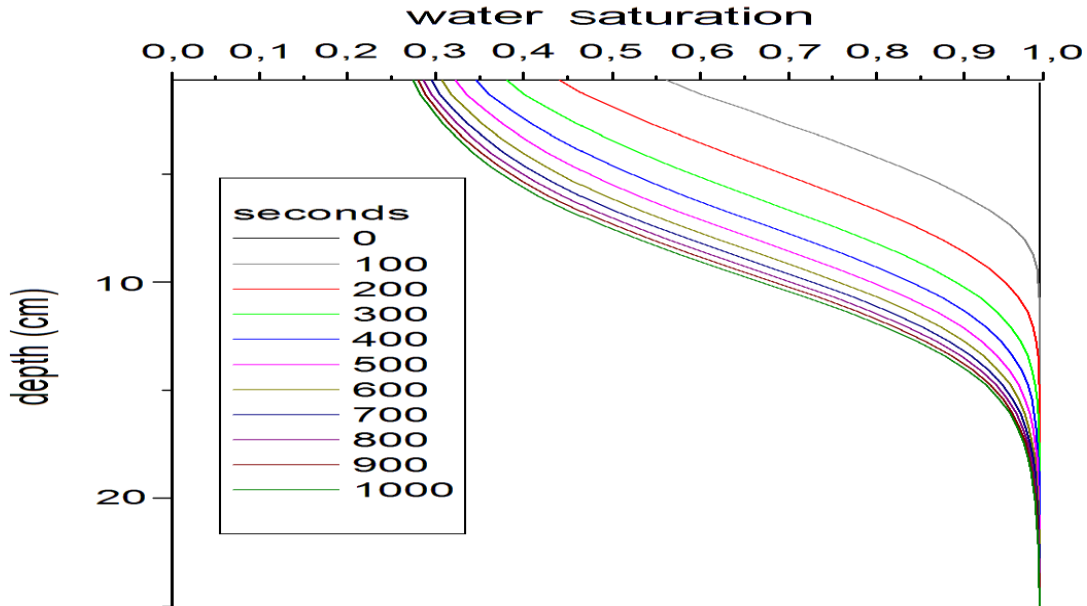


**Figure 1:** The drainage problem statement

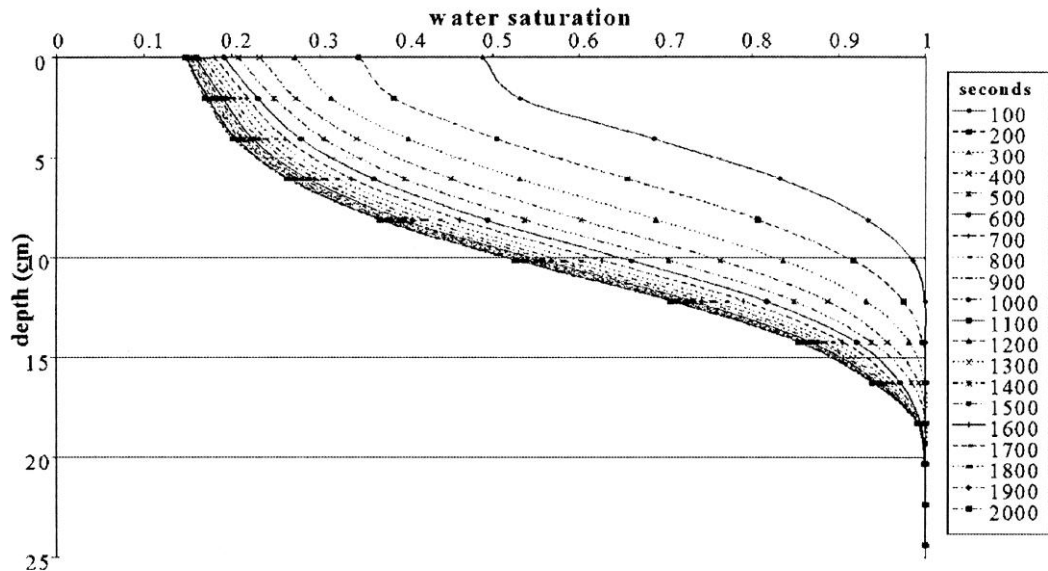
Initially the given thin column is filled by a fully water-saturated porous medium. Sources are absent, pumping of fluids does not occur. At the initial moment the hydrostatic distribution of the water pressure is set in the column, the air pressure is assumed to be equal to the water pressure. The top boundary is open to the atmosphere ( $P_g = \text{const}$ ) with a no-flow

condition on water, a no-flow condition on air is set at the bottom, only water drains from the column ( $P_w = \text{const}$ ). All physical quantities are as in [5], the medium is homogeneous. The small parameters are chosen empirically. In the current computation they equal:  $l = 10^{-7}$  cm,  $\tau = 10^{-3}$  s (that coincides with the time step  $\Delta t = 10^{-3}$  s at the spatial grid step  $h = 0.67$  cm).

The obtained distribution of water saturation with the depth at different time moments is depicted in Figure 2.



**Figure 2:** Distribution of water saturation in depth at certain points in time for the drainage problem (solution via the model and algorithm from Section 3.1)



**Figure 3:** Distribution of water saturation in depth at certain points in time for the drainage problem (Pinder&Gray solution [5])

The solution (see Figure 2) is smooth due to the regularizer. It is found that the employed three-level scheme for the modified continuity equation allows increasing the time step by an order of magnitude in comparison with the two-level upwind scheme for the classical parabolic equation.

Figure 3 is taken from [5]: the authors indicate that the results were obtained numerically using the NAPL Simulator program (freely available, <https://www.epa.gov/water-research/non-aqueous-phase-liquid-napl-simulator>).

A rather good agreement is observed at the comparison of figures 2 and 3 that testifies to the adequacy of the developed kinetic approach to porous medium flow simulation.

#### 4 AN APPROACH WITH THE MASS FLUX RELAXATION

Let us consider another approach to deriving hyperbolized equations which seems to be physically more reasonable. Equation (1) can be briefly written in the form:

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \operatorname{div} \mathbf{Q}_\alpha = q_\alpha, \quad \alpha = w, n \quad (12)$$

where  $\mathbf{Q}_\alpha$  is the  $\alpha$ - phase flux.

Let  $\mathbf{Q}_\alpha^D = \rho_\alpha \mathbf{u}_\alpha$  be the Darcy flux. In the classical model:  $\mathbf{Q}_\alpha = \mathbf{Q}_\alpha^D$ .

Let us now introduce the flux relaxation:

$$\mathbf{Q}_\alpha = \mathbf{Q}_\alpha^D - \tau \frac{\partial \mathbf{Q}_\alpha}{\partial t} \quad (13)$$

The small parameter  $\tau$  is the relaxation parameter characterizing the time of equilibrium establishing in the system.

The following expression is valid:

$$\operatorname{div} \mathbf{Q}_\alpha = \operatorname{div} \mathbf{Q}_\alpha^D - \tau \operatorname{div} \frac{\partial \mathbf{Q}_\alpha}{\partial t} \quad (14)$$

If to differentiate equation (12) by time, then to multiply it by  $\tau$ , to take into account (14) and to substitute  $\operatorname{div} \mathbf{Q}_\alpha$  expressed from (5), one can obtain the next final form of the continuity equation modified by the flux relaxation introduction:

$$\tau \frac{\partial^2(\phi\rho_\alpha S_\alpha)}{\partial t^2} + \frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \operatorname{div} \mathbf{Q}_\alpha^D = q_\alpha + \tau \frac{\partial q_\alpha}{\partial t} \quad (15)$$

The known technique used in [6] to get the system of equations suitable for implementation by IMPES (IMplicit Pressure – EXplicit Saturation) method [6, 4] can be also applied to the model including the modified equation (15). The purpose is to turn the model into the formulation in terms of the average pressure and the water saturation.

If to divide (15) by  $\rho_\alpha$  and to summarize these two equations for the phases, to substitute the Darcy velocity, to account for the capillary pressure and then to make some simplifications ( $\phi = \text{const}$ , the state equations are linear) the next pressure equation is derived:

$$\begin{aligned}
 & \frac{1}{\rho_n} \operatorname{div}(\rho_n \lambda_n \operatorname{grad} P_{avg}) + \frac{1}{\rho_w} \operatorname{div}(\rho_w \lambda_w \operatorname{grad} P_{avg}) + \\
 & + \frac{1}{2} \left[ \frac{1}{\rho_n} \operatorname{div}(\rho_n \lambda_n \operatorname{grad} P_c) + \frac{1}{\rho_w} \operatorname{div}(\rho_w \lambda_w \operatorname{grad} P_c) \right] + q_t = \\
 & = \phi(S_n c_n + S_w c_w) \left( \frac{\partial P_{avg}}{\partial t} + \tau \frac{\partial^2 P_{avg}}{\partial t^2} \right) + \\
 & + \frac{1}{2} \phi(S_n c_n - S_w c_w) \left( \frac{\partial P_c}{\partial t} + \tau \frac{\partial^2 P_c}{\partial t^2} \right) + \\
 & + g \left[ \frac{1}{\rho_n} \operatorname{div}(\rho_n^2 \lambda_n \operatorname{grad} z) + \frac{1}{\rho_w} \operatorname{div}(\rho_w^2 \lambda_w \operatorname{grad} z) \right] + \\
 & + 2\tau \phi \left( c_n \frac{\partial S_n}{\partial t} + c_w \frac{\partial S_w}{\partial t} \right) \frac{\partial P_{avg}}{\partial t} + \\
 & + \tau \phi (c_n + c_w) \frac{\partial S_w}{\partial t} \frac{\partial P_c}{\partial t}
 \end{aligned} \tag{16}$$

The equation for the water saturation is as follows:

$$\begin{aligned}
 \operatorname{div}(\rho_w \lambda_w \operatorname{grad} P_w) + q_w & = g \cdot \operatorname{div}(\rho_w^2 \lambda_w \operatorname{grad} z) + \phi \rho_w S_w c_w \frac{\partial P_w}{\partial t} + \\
 & + \phi \rho_w \frac{\partial S_w}{\partial t} + \tau \phi \rho_w \frac{\partial^2 S_w}{\partial t^2} + \tau \phi \rho_w S_w c_w \frac{\partial^2 P_w}{\partial t^2} + \\
 & + 2\tau \phi \rho_w c_w \frac{\partial P_w}{\partial t} \frac{\partial S_w}{\partial t}
 \end{aligned} \tag{17}$$

The listed below notations are used:

$$\begin{aligned}
 q_t & = \frac{q_n}{\rho_n} + \frac{q_w}{\rho_w}, \quad c_n = \frac{1}{\rho_n} \frac{d\rho_n}{dP_n}, \quad c_w = \frac{1}{\rho_w} \frac{d\rho_w}{dP_w}, \quad P_{avg} = \frac{P_n + P_w}{2}, \quad P_n = P_{avg} + \frac{P_c}{2}, \quad P_w = P_{avg} - \frac{P_c}{2}, \\
 \lambda_n & = -\frac{Kk_n}{\mu_n}, \quad \lambda_w = -\frac{Kk_w}{\mu_w}.
 \end{aligned}$$

Both equations (16), (17) contain second time derivatives with the small parameter.

A fully explicit algorithm is proposed for the numerical implementation of the modified model. Three-level explicit difference schemes are employed for the approximation wherein relative phase permeabilities are calculated upwind. First,  $P_{avg}^{j+1}$  is found from the scheme for (16), time derivatives of saturations in this scheme are calculated explicitly using values from the previous time level. Second,  $S_w^{j+1}$  is found from the scheme for (17) using

$$P_w = P_{avg}^{j+1} - \frac{P_c(S_w^j)}{2}.$$

## 5 TEST PREDICTIONS

A test problem on two-phase water/oil flow is predicted to verify and to compare the proposed approaches to porous medium flow simulation. The investigated domain of a homogenous isotropic porous medium is a parallelepiped of the size  $1\text{ m} \times 1\text{ m} \times 5\text{ m}$ . Due to the symmetry the problem is reduced to a 1D geometry. The space step of the grid is fixed as  $h = 0.05\text{ m}$ .

Initial conditions:  $S_w = 0.35$ ,  $P_{avr} = -0.1z + 1.5$

Boundary conditions:  $S_w|_{z=0} = 0.7$ ,  $S_w|_{z=5} = 0.35$ ,  $P_{avr}|_{z=0} = 1.5\text{ atm}$ ,  $P_{avr}|_{z=5} = 1\text{ atm}$

Table 1 contains fluid and medium parameters used in computations.

**Table 1:** Fluid and medium parameters

Physical quantity	Water, $w$	Oil, $n$
Density reference value, $\text{kg}/\text{m}^3$	1000	850
Dynamic viscosity, $\text{Pa} \cdot \text{s}$	$10^{-3}$	$10^{-2}$
Compressibility, $\text{Pa}^{-1}$	$4.4 \cdot 10^{-10}$	$10^{-9}$
Residual saturation	0.05	0.05
Pressure reference value, atm	1	1
Porosity	0.4	
Absolute permeability, $\text{m}^2$	$6.64 \cdot 10^{-11}$	

The next parameters are assigned in (5), (6) :  $N = 3.25$ ,  $\alpha = 10$ .

The system (1)-(7) is strongly non-linear therefore it does not seem possible to obtain the exact solution analytically. As a reference solution of the test problem the solution of system (1)-(7) obtained by IMPES method [6, 4] with the time step  $\Delta t = 10^{-4}\text{ s}$  is taken. The time step is selected by comparing results of calculations with different steps. Further reduction of the step does not lead to a significant change in the results. The detailed data are presented in Table 2 which reports errors of IMPES method at time moments of 50 and 100 seconds for different time steps. These errors are calculated relative to the solution obtained with  $\Delta t = 10^{-4}\text{ s}$ . The relative error between quantities  $A$  and  $B$  is given by the next formula:

$$\varepsilon = \sqrt{\sum_{i=1}^{N_i} \left( \frac{A_i - B_i}{A_i} \right)^2} / N_i \quad (18)$$

**Table 2:** Errors of IMPES method at calculations of  $P_{avr}$  and  $S_w$  with different time steps

$\Delta t, \text{ s}$	$\varepsilon_p, \varepsilon_s$ at $t = 50 \text{ s}$	$\varepsilon_p, \varepsilon_s$ at $t = 100 \text{ s}$
$1 \cdot 10^{-2}$	$1.4 \cdot 10^{-7}$ , $4.1 \cdot 10^{-6}$	$1.0 \cdot 10^{-7}$ , $2.8 \cdot 10^{-6}$
$1 \cdot 10^{-3}$	$2.7 \cdot 10^{-8}$ , $7.8 \cdot 10^{-7}$	$3.0 \cdot 10^{-8}$ , $5.4 \cdot 10^{-7}$
$5 \cdot 10^{-4}$	$1.5 \cdot 10^{-8}$ , $4.2 \cdot 10^{-7}$	$1.7 \cdot 10^{-8}$ , $3.0 \cdot 10^{-7}$
$2 \cdot 10^{-4}$	$4.7 \cdot 10^{-9}$ , $1.3 \cdot 10^{-7}$	$5.8 \cdot 10^{-9}$ , $9.3 \cdot 10^{-8}$



While solving the test problem by the model and the algorithm proposed in Section 4 the small parameter  $\tau$  is chosen empirically depending on the time step to ensure the stability of computations. Comparison of the reference solution with the solution obtained via the modified model implemented by three-level explicit schemes is reflected in Table 3.

**Table 3:** Errors of the three-level scheme relative to the reference solution for different  $\Delta t$  and  $\tau$  at  $t = 20$  s

$\Delta t, s$	$\tau, s$	$\varepsilon_p$	$\varepsilon_s$
$1 \cdot 10^{-4}$	$1 \cdot 10^{-5}$	$3.2 \cdot 10^{-4}$	$2.8 \cdot 10^{-3}$
$1 \cdot 10^{-4}$	$2 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$
$1 \cdot 10^{-4}$	$5 \cdot 10^{-5}$	$1.9 \cdot 10^{-7}$	$2.3 \cdot 10^{-6}$
$1 \cdot 10^{-4}$	$1 \cdot 10^{-4}$	$3.1 \cdot 10^{-7}$	$3.7 \cdot 10^{-6}$
$1 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$5.3 \cdot 10^{-7}$	$6.5 \cdot 10^{-6}$
$2 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$2.4 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$
$2 \cdot 10^{-4}$	$5 \cdot 10^{-4}$	$6.3 \cdot 10^{-7}$	$8.0 \cdot 10^{-6}$

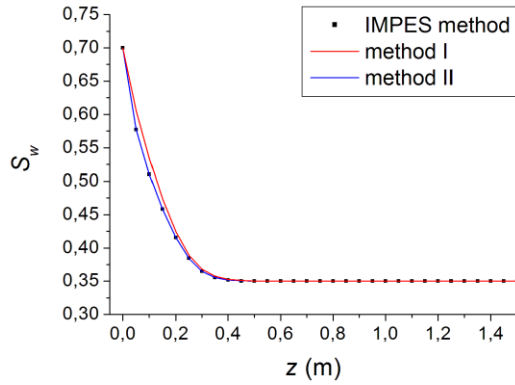
The error  $\varepsilon_s > 10^{-3}$  is too large, the scheme is unstable at the corresponding values of  $\Delta t$  and  $\tau$ . For long-term calculations the time step and the relaxation time are chosen as follows:  $\Delta t = 10^{-4}$  s,  $\tau = 10^{-4}$  s. Note that the two-level explicit scheme implementing the classical model with the parabolic continuity equation is stable at  $\Delta t \leq 10^{-5}$  s. Thus the hyperbolization allows increasing the time step of explicit methods at least by an order of magnitude.

The same conclusion is drawn while solving the test problem by the model and the algorithm proposed in Section 3.1: values  $\Delta t = 10^{-4}$  s,  $\tau = 10^{-4}$  s prove to be optimal. Consideration of a number of test problems shows that the choice  $\Delta t = \tau$  leads to satisfactory results. The choice of the regularizing parameter  $l$  is more difficult because it affects not only the stability but also the accuracy of the method. Good results for the above test are achieved when  $l = 10^{-8}$  m.

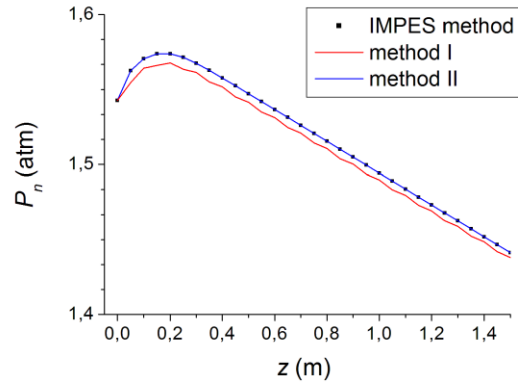
Figure 4 illustrates the comparison of the water saturation and the oil pressure obtained at two time moments by different methods: the approach from Section 3.1 is marked as “method I”, the approach from Section 4 is called “method II”, the reference solution corresponds to “IMPES method”. A very good agreement is observed.

## 6 CONCLUSIONS

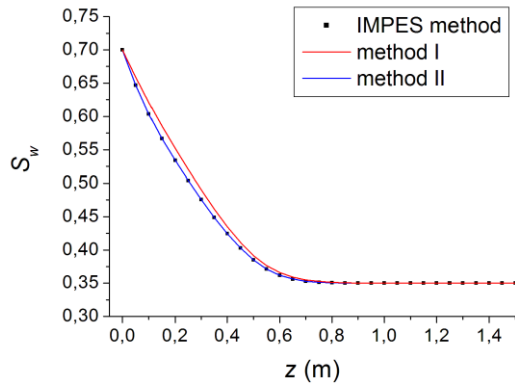
The proposed approaches to the simulation of compressible fluid flow in porous media use a hyperbolized continuity equation and its approximation by an explicit difference scheme. The algorithms provide the same increase in the time step and are similar in terms of computational costs. At implementation of the QGD-based approach there are difficulties in choosing the regularization parameter that significantly affects the accuracy. The second approach is more in line with traditional methods. The hyperbolization in this case seems to be physically reasonable. However this algorithm is more difficult to generalize for predicting multiphase multicomponent fluid flows. The both approaches will be further developed for solving applied problems using supercomputers.



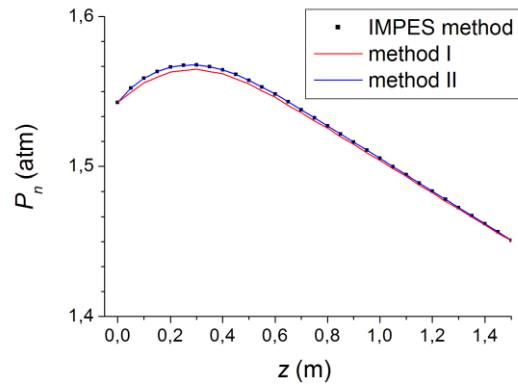
(a) Water saturation,  $t = 100$  s



(b) Oil pressure,  $t = 100$  s



(c) Water saturation,  $t = 300$  s



(d) Oil pressure,  $t = 300$  s

**Figure 4:** Distributions of water saturation and oil pressure in depth at different time moments for the two-phase water/oil test problem

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