About one discrete model of splitting by the physical processes of a piezoconductive medium with gas hydrate inclusions

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Abstract. The thermodynamically equilibrium model for splitting by the physical processes of a two-component three-phase filtration fluid dynamics with gas hydrate inclusions is considered in the paper, for which a family of two-layer completely conservative difference schemes of the support operators method with time weights profiled in space is constructed. On the irregular grids of the theory of the support-operators method applied to the specifics of the processes of transfer of saturations and internal energies of water and gas in a medium with gas hydrate inclusions, methods of directwind approximation of these processes are considered. These approximations preserve the continual properties of divergence–gradient operations in their difference form and are related to the velocity field providing saturations transfer and internal energies of fluids. Fluid dynamics with gas hydrate inclusions are also calculated on the basis of the proposed approach, in particular, in areas of severe pressure depression in the collector space.

1. Introduction

Many porous materials, saturated with a fluid or a mixture of fluids, undergo physical-chemical transformations of the solid phase. For example, gas hydrates, which are compounds of gas and water molecules, can be mentioned. In the initial state, the pore space is completely or partially filled with hydrates in the solid state at low temperature and high pressure. When the temperature rises and the compression level decreases, the hydrate decomposes into gas and water. A decrease in temperature and an increase in pressure lead to the formation of hydrates. Huge hydrocarbon reserves in gas hydrate deposits can be extracted quite fully only with the use of mining technologies based on physicochemical transformations of the porous medium, which indicates the relevance of studying such transformations.

Our common goal is to model the hydrodynamic, geomechanical and physical-chemical processes that occur during the development and study of gas hydrate deposits. They are usually porous layers saturated with hydrates, water and hydrocarbon gases. The goal is to
optimize the production of hydrocarbon raw materials from gas hydrate deposits, ensure safety of work with gas hydrates and solve related ecological problems.

In the world, several computational codes have been developed to calculate the fluid dynamics in the reservoir, taking into account gas hydrates, for example CMG STARS, STOMP-HYD, TOUGH+HYDRATE, developed by Lawrence Berkeley National Laboratory, USA, MH21-HYDRES [1], created as part of the national hydrate program in Japan with the support of a number of scientific and commercial organizations, etc.

The methods are based on different approaches, each of which has certain advantages and disadvantages. International research, based on the National Energy Technology Laboratory and the U.S. Geological Survey (USA) [2], is conducted for their comparison. New methods are constantly appearing, for example, in Germany—SUGAR based on PetroMod [3], in Norway—RetrasoCodeBright (RCB) [4]. However, the published work does not describe in detail the methodology for the joint solution of equations system. Therefore, the development of domestic mathematical models and software for solving similar problems is an actual task.

In the works [5, 6], a model of two-component three-phase fluidodynamics in porous media with gas hydrate inclusions was proposed and numerically studied. The model was based on splitting of the initial balance principles of the problem (i.e. the conservation of masses of fluid components and of the total energy of the system) by the physical processes into the block of the fluids saturations transfer against the background of a given velocity field (possessing mainly hyperbolic properties), and a piezoconductive block of the system with hydrate inclusions, which determines the dissipative evolution of the thermodynamic parameters of the equilibrium fluid-hydrate model. Such a splitting by physical processes makes it possible to create effective applied computational algorithms that use a large time step, which is impossible within the framework of the model of the initial balance principles with the combined matrix of a system with mixed hyperbolic and multiscale parabolic properties. The implementation of an unsplit physical process using an implicit scheme in this case would lead to an increase in the total number of unknown variables \((P, S_w, S_v)\) and the use of a non-self-adjoint undefined matrix of the corresponding algebraic system of equations.

In the present work, a discrete model of splitting is proposed with obtaining the corresponding piezoconductive equation for a fluid-dynamic environment with gas-hydrate inclusions. It is important that the split model thus obtained is differentially equivalent to the discrete first balance principles of the system, written in a divergent form. This approach to the creation of completely conservative schemes in the studied fluid-hydrate medium required the introduction of a special free-volume non-linear approximation of the grid functions in time, which depends on the volume fraction in the pores occupied by the fluids and is easy to implement. Also, methods of directwind approximation of saturations transfer processes in a medium with gas-hydrate inclusions along with the simultaneous preservation of the continuum properties of \(\text{divgrad} = \nabla \cdot \nabla\) operations in their difference form associated with the velocity field providing this transfer were examined in work on the grids of the theory of the support-operators method [7, 8].

2. Formulation of the problem

In a spatial domain \(O\) with a boundary \(\partial O\), we consider thermodynamically equilibrium two-component (water, methane) three-phase equations of filtration fluid dynamics with gas-hydrate inclusions [5]:

\[
\frac{\partial}{\partial t} \{ m [ S_v S_w \rho_w + (1 - S_v) \rho_v \beta_w ] \} + \nabla \cdot [ \rho_w \mathbf{V}_w ] + q_w = 0,
\]

\[
\frac{\partial}{\partial t} \{ m [ S_v (1 - S_w) \rho_g + (1 - S_v) \rho_v (1 - \beta_w) ] \} + \nabla \cdot [ \rho_g \mathbf{V}_g ] + q_g = 0,
\]
\[ V_w = -\frac{k_{lw}}{\mu_w} (\nabla P - g \rho_w k), \] (3)
\[ V_g = -\frac{k_{lg}}{\mu_g} (\nabla P - g \rho_g k), \] (4)
\[
\frac{\partial}{\partial t} \left\{ m \left[ S_v (S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \varepsilon_g) + (1 - S_v) \rho_v \varepsilon_v \right] + (1 - m) \rho_s \varepsilon_s \right\} + \nabla \cdot \left\{ \rho_w \varepsilon_w V_w + \rho_g \varepsilon_g V_g + [P(V_w + V_g)] \right\} + \nabla \cdot W + q_e = 0, \] (5)
\[ W = -m [S_v (S_w \lambda_w + (1 - S_w) \lambda_g) + (1 - S_v) \lambda_v] + (1 - m) \lambda_s \nabla T, \] (6)
\[ T_{\text{dis}} = f(P) \] (7)

(with certain boundary conditions) along with the integral relation
\[
\int_{0}^{t} (X \nabla u) \, dV + \int_{0}^{t} u \nabla \cdot X \, dV = \int_{\partial \Omega} u (X, ds). \] (8)

Here, the indices \( g, w, \nu \) and \( s \) refer to the gas, water, hydrate and skeleton of porous medium; \( t \) is the index indicating the phase; \( P \) is the pressure, \( S_w \) is the water saturation, \( \nu \) is the hydrate saturation, \( S_v = 1 - \nu \) is the thawing, \( \rho_l(P,T) \) and \( \varepsilon_l(P,T) \) are the densities and internal energies of the unit mass of the phases, \( V_l \) is the filtration rate of the corresponding phase; \( \beta_w \) is the mass fraction of water in the hydrate, \( r \) is the radius vector, \( t \) is the time, \( q_w, q_g \), and \( q_\nu \), depending on the parameters \( t, r, S_w, S_\nu, P \) of the respective sources density; \( k(r, S_\nu, P) \) is absolute permeability, \( k_{lw}(S_w), k_{lg}(S_w) \) are relative permeabilities, \( \mu_w, \mu_g \) are viscosities of gas and water, \( g \kappa \) is the vector of acceleration of gravity, directed vertically downwards. \( W \) is heat flow, \( \lambda_l(P,T) \) are coefficients of thermal conductivity. According to the Gibbs phase rule, the three-phase two-component hydrate system is multivariant, i.e. has one degree of freedom (temperature or pressure) [9]. Consequently, for a gas hydrate that is in equilibrium with liquid water or ice, the dependence \( T_{\text{dis}} = f(P) \) is unambiguous; \( u \) and \( X \) are arbitrary scalar (temperature, pressure, internal energy, etc) and vector physically related to the gradient flow of this scalar quantity.

The enthalpies \( u = \varepsilon_l + P/\rho_l \) of hydrate, free water and gas are thermodynamically consistent in the sense of the following relation
\[ \beta_w i_w + (1 - \beta_w) i_\nu = i_\nu + h, \] (9)
where \( h \) is the latent heat of the phase transition of a unit of hydrate mass. For specific (per unit mass) phase enthalpies is also valid [10]
\[ di_l = c_{pl} \left(-k_{dl} dP + dT \right) \] (10)
with throttling coefficients
\[ k_{dl} = \frac{1}{c_{pl}} \left[ T \left( \frac{\partial V_l}{\partial T} \right)_p - V_l \right]. \] (11)

Here \( c_{pl} \) and \( V_l = 1/\rho_l \) are the specific heat capacities (at constant pressure) and the volumes of the phases. In particular, for a gas phase with the equation of state
\[ \rho_g = \frac{P}{z_g RT}. \] (12)
Justly
\[ k_{lg} = \frac{RT^2}{c_{pg} P} \frac{\partial z_g}{\partial T}. \] (13)
which means the presence of the Joule–Thomson effect \( k_{IG} \neq 0 \) for a nonideal gas with a coefficient of supercompressibility \( z_g \) in the studied processes of nonisothermal filtration.

From equations (1), (2), (5), an equation for the three-phase piezoconductive of fluid dynamics with hydrate inclusions can be obtained in the following form [5]:

\[
m \delta_c \left\{ S_v \left[ S_w \left( \frac{\rho_w}{\rho_v} \right)_t + \left( 1 - S_w \right) \frac{\left( \rho_g \right)_t}{\rho_g} \right] \right. \left. + \left( 1 - S_v \right) \frac{\left( \rho_v \right)_t}{\rho_v} + \frac{\left( m \right)_t}{m} \right\} + \frac{\psi}{m \rho_v} \{ m \} \{ S_v \left[ S_w \rho_w (\varepsilon_w)_t + \left( 1 - S_w \right) \rho_g (\varepsilon_g)_t \right] + \left( 1 - S_v \right) \rho_v (\varepsilon_v)_t \} + \left[ \left( 1 - m \right) \rho_s \varepsilon_s \right]_t \}
\]

\[
\begin{align*}
\delta_c \text{DIG} + \frac{\psi}{m \rho_v} \text{DIG}_c &= 0, \\
\text{DIG}_c &= [\nabla \cdot \left( \rho_w \varepsilon_w \mathbf{V}_w \right) - \varepsilon_w \nabla \cdot \left( \rho_w \mathbf{V}_w \right)] + [\nabla \cdot \left( \rho_g \varepsilon_g \mathbf{V}_g \right) - \varepsilon_g \nabla \cdot \left( \rho_g \mathbf{V}_g \right)] \\
&+ \nabla \cdot [P(\mathbf{V}_w + \mathbf{V}_g)] + \nabla \cdot \mathbf{W} + (q_e - \varepsilon_w q_w - \varepsilon_g q_g) \\
&= \rho_w \mathbf{V}_w \nabla \varepsilon_w + \rho_g \mathbf{V}_g \nabla \varepsilon_g + \nabla \cdot [P(\mathbf{V}_w + \mathbf{V}_g)] + \nabla \cdot \mathbf{W} \\
&+ (q_e - \varepsilon_w q_w - \varepsilon_g q_g).
\end{align*}
\]

Here

\[
\frac{\psi}{m \rho_v} = \left( \phi - \frac{1}{\rho_v} \right) \geq 0, \quad \phi = \frac{\beta_w}{\rho_w} + \frac{\left( 1 - \beta_w \right)}{\rho_g},
\]

\[
\delta_c = \beta_w \varepsilon_w + \left( 1 - \beta_w \right) \varepsilon_g - \varepsilon_v \geq 0
\]

are respectively specific jumps (per unit mass) for the phase transition of the volume and internal energy. The notation is also used hereinafter

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial t}, \quad \frac{\partial}{\partial P} = \frac{\partial}{\partial P}.
\]

Equation (14) is the main piezoconductive-dissipative thermodynamic equilibrium relation of three-phase two-component fluid dynamics with hydrate inclusions physically split with the saturation block (1)–(4) possessing mainly hyperbolic properties on the background of the fixed thermodynamic parameters of the medium [5]. Let us introduce a new value—the intensity of the hydrate system \( D_p \) by the relation

\[
D_p = m \delta_c \left\{ S_v \left[ S_w \left( \frac{\rho_w}{\rho_v} \right)_p + \left( 1 - S_w \right) \frac{\left( \rho_g \right)_p}{\rho_g} \right] \right. \left. + \left( 1 - S_v \right) \frac{\left( \rho_v \right)_p}{\rho_v} + \frac{\left( m \right)_p}{m} \right\} + \frac{\psi}{m \rho_v} \{ m \} \{ S_w \left[ S_w \rho_w (\varepsilon_w)_p + \left( 1 - S_w \right) \rho_g (\varepsilon_g)_p \right] + \left( 1 - S_v \right) \rho_v (\varepsilon_v)_p \} + \left[ \left( 1 - m \right) \rho_s \varepsilon_s \right]_p
\]

\[
\begin{align*}
\frac{\partial}{\partial t}
\end{align*}
\]

and we rewrite equation (14) in a more compact form

\[
D_p \frac{\partial P}{\partial t} + \delta_c \text{DIG} + \frac{\psi}{m \rho_v} \text{DIG}_c = 0.
\]

In equation (19), we take the total derivative with respect to pressure, taking into account the dependence (7). Using this dependence (7) and choosing the corresponding internal energies \( \varepsilon_w \) and \( \varepsilon_g \) as the unique thermodynamic degree of freedom in equations (3), (4), (14)–(16), we obtain the equation (14) in the energy representation.
3. Grids of the support-operators method

The presence of a closed conjugate (shifted) grid, consisting, for example, of domains \( d(\omega) \) around nodes \( \omega \) (figure 1) is characteristic for grids of this type, consisting of cells \((\Omega)\) formed by nodes \((\omega)\), faces \(\sigma\) and edges \(\lambda\).

The metric grid operator \( \sigma(\lambda) = \sum_{\phi(\lambda)} V_{\phi} e'_{\phi}(\lambda) \) (see also below) determines the boundaries of the node domain. Here the bases \( \phi(\lambda) \) enter pairwise in the cells \( \Omega(\lambda) \) adjacent to the edge \(\lambda\). Calibration of the difference grid consists in choosing the volumes of bases (with the natural normalization condition \( \sum_{\phi(\lambda)} V_{\phi} = V_\Omega \)). It defines the construction of a closed conjugate mesh for various classes of grids. These are triangular-quadrangular 2D meshes, tetrahedral, parallelepipedal, prismatic, etc. 3D grids, as well as their mortar stitching, adaptation (with the introduction of new nodes in cells \(\Omega\)) with the preservation of self-adjointness and the sign-definiteness of the corresponding divergence–gradient operations of vector analysis of continual boundary value problems. The rest of the presentation is of a general nature, a specific choice of local basis volumes \( V_{\phi} \) is illustrated by the example of a triangular-quadrangular 2D grid.

In the region \( O \) we introduce a family of irregular difference grids. We confine ourselves to the case when the grid consists of triangular and quadrangular cells \((\Omega)\), bases \((\phi)\), nodes \((\omega)\), edges \((\lambda)\), and associated with them the boundaries of the nodal balance domains \( d(\omega) \) (see figure 1).

The bases \( \phi \) are created by the system of initial (covariant) unit vectors \( e(\lambda) \) formed by the edges. By the centers of cells \( \Omega \) and edges \(\lambda\) we mean the arithmetic mean radius vectors of the nodes \(\omega\) of their generators. The curve that connects these centers (two adjacent cells through an edge or a cell with a boundary edge \(\partial\lambda\)) is a surface

\[
\sigma(\lambda) = \sum_{\phi(\lambda)} v_{\phi} e'_{\phi}(\lambda)
\]

oriented as well as the unit vector \( e(\lambda) \). Here \( e'_{\phi}(\lambda) \) are the unit vectors of the reciprocal (contravariant) bases with respect to the initial bases \( e(\lambda) \). The base volume is given by the formula \( v_{\phi} = \frac{1}{6}[e(\lambda_1) \times e(\lambda_2)] \) for a triangular cell \(\Omega\) containing a basis \( \phi \) and \( v_{\phi} = \frac{1}{4}[e(\lambda_1) \times e(\lambda_2)] \) for a quadrangular cell, if \( \lambda_1(\phi) \) and \( \lambda_2(\phi) \) are the edges forming the basis \( \phi \). Finally, \( \sum_{\phi(\lambda)} \) is summation over all bases \( \phi \) in whose formation the edge \(\lambda\) took part. The surfaces \( \sigma(\lambda(\omega)) \) closed around the node \(\omega\) form nodal domains \( d(\omega) \).

The internal divergence of a vector field \( D W_X : (\phi) \rightarrow (\omega) \) is defined by approximating the Gauss theorem on \( d(\omega) \):

\[
D W_X = \sum_{\lambda(\omega)} s_{\lambda(\omega)} X_{\lambda}(\lambda),
\]

\[
X_{\lambda}(\lambda) = \sum_{\phi(\lambda)} v_{\phi} (e'_{\phi}(\lambda), X_{\phi}),
\]

\[
e'_{\phi}(\lambda) = W_{\phi}(\lambda) e'_{\phi}(\lambda).
\]

Here and below \( f : (X) \rightarrow (Y) \) denotes an operator acting from the field \( X \) to the field \( Y \); \( \sum_{\lambda(\omega)} \) is the summation over all edges having a common node \(\omega\).

The grid vector field \( X \) is given by its representations in the bases \( X_{\phi} \). The multipliers \( W_{\phi}(\lambda) > 0 \) given in the bases \(\phi\) on the ribs \(\lambda(\phi)\) formed them are related to the directwind monotonization of the approximation of the transfer processes existing in the medium. For the sake of convenience, let us introduce the term contravariant directwind for these factors. The absence of an index, here denoted as \( W \) in expressions \( D W_X, X_{\phi}(\lambda), e'_{\phi}(\lambda) \) and \( GRAD_WU \) automatically denotes \( W_{\phi}(\lambda) = 1 \) in all bases \(\phi\) on the edges \(\lambda(\phi)\) forming them, i.e. means the absence of contravariant directwind in the approximations used.
Denoting by \((\cdot)_{\Delta}\) of the corresponding differential expressions approximation, we have:

\[
\left( \int_{\Omega} (X, \nabla u) dv \right)_{\Delta} = -\left( \int_{\Omega} u \nabla \cdot X dv - \int_{\partial \Omega} u(X, ds) \right)_{\Delta} = -\sum_{\omega}(u_{\omega}, \text{DIN}_W X)
\]

\[
= \sum_{\phi} v_{\phi}(X_{\phi}, \text{GRAD}_W u).
\]

A gradient vector field \(\text{GRAD}_W : (\omega) \rightarrow (\phi)\) is given by its representations in bases

\[
\text{GRAD}_W u = \sum_{\lambda(\phi)} \Delta_{\lambda} u e_{W_{\phi}}(\lambda), \quad \Delta_{\lambda} u = -\sum_{\omega(\lambda)} s_{\lambda}(\omega)u_{\omega} = u_{\omega^*} - u_{\omega}.
\]

Assuming in the bases \(\phi\) as \(X_{\phi}\) a vector field \(X_{W_{\phi}} = K_{\phi}\text{GRAD}_W u\), we obtain a self-adjoint nonnegative operator \(-\text{DIN}_W X_{W_{\phi}} : (\omega) \rightarrow (\omega)\) or \(-\text{DIN}_W K\text{GRAD}_W : (\omega) \rightarrow (\omega)\). Here the flow vector field \(X_{W_{\phi}}\) is given by its components in the bases \(X_{W_{\phi}}\). It is determined by the gradient properties of the scalar grid function \(u\), given at the nodes \(\omega\) and the grid symmetric positive definite tensor field of conductivity \(K\), given by their representations in the bases \(K_{\phi}\).

This operator will be strictly positive if at least one boundary node of the connected difference grid will be given the first boundary value problem, i.e. the scalar grid function vanishes in this boundary node.

It is believed that, as the approximation is increased, the factors of contravariant directwind tend to be single, i.e. \(W_{\phi}(\lambda) \rightarrow 1\). Moreover, the operator \(-\text{DIN}_W K\text{GRAD} : (\omega) \rightarrow (\omega)\) becomes close to a self-adjoint nonnegative operator \(-\text{DIN}_W K\text{GRAD} : (\omega) \rightarrow (\omega)\), although in the strict sense (with the exception of an orthogonal grid) is not self-adjoint and nonnegative.

Cells consisting of orthogonal bases do not violate the properties of self-adjointness and sign-definiteness of the operator \(\text{DIN}_W \text{GRAD}\) in the strict sense, in spite of the presence in their bases of approximate contravariant directwind.

To preserve the properties of self-adjointness and the sign-definiteness of this operator, we consider two families of approximations:

(i) Schemes with limited directwind. We select the set of grid cells \((\Omega^*)\) in which there is at least one non-orthogonal basis \(\phi\) formed by the edges \((\lambda(\phi))\). In all bases \((\phi(\Omega^*))\) within these cells \(\Omega^*\) (i.e., can be orthogonal) is considered \(W_{\phi}(\lambda) = 1\). I.e. in these bases there is no contravariant directwind. For example, the dependence of the representation of the tensor field of conduction \(K_{\phi}\) on “hyperbolic” variables (here are thawing \(S_{\nu}\), water saturation \(S_{\omega}\), etc) is approximated directly at the central site \(\omega\) of the grid forming the basis \(\phi\). Such schemes will have a self-adjoint and a sign-definite operator \(\text{DIN}_W K\text{GRAD} : (\omega) \rightarrow (\omega)\). However, they do not monotonize on the set of grid cells containing non-orthogonality.

(ii) Quasi-directwind schemes. We denote the set of non-orthogonal grid bases by \((\phi^*)\). Correspondingly, \((\phi)/(\phi^*)\) are orthogonal bases. To approximate a vector field \(X = K\nabla u\),
we introduce
\[ X_W = K_{\phi} \text{GRAD}^*_W u, \quad \text{GRAD}^*_W u = \left\{ \begin{array}{ll}
\text{GRAD} u, & \phi \in (\phi) \\
\text{GRAD}^*_W u, & \phi \in (\phi^*)
\end{array} \right. \]

These schemes will also have a self-adjoint and sign-definite operator \( D_{W} K \text{GRAD}^*_W : (\omega) \to (\omega) \). Since, with increasing approximation, the factors of contravariant directwind tend to unit ones, i.e. \( W_{\phi}(\lambda) \to 1 \), then the operators \( \text{GRAD}^*_W : (\omega) \to (\phi) \) and \( \text{GRAD} : (\omega) \to (\phi) \) approximate the differential operator \( \nabla \). In contrast to schemes with limited directwind, quasi-directwind schemes, along with self-adjointness and the sign-definiteness of the operator \( D_{W} K \text{GRAD}^*_W : (\omega) \to (\omega) \) in nonorthogonal grid bases \( (\phi^*) \), preserve monotonicity in the “main” sense when calculating flows in conjugate basis directions.

Approaches (i) and (ii) can be applied locally, i.e. only in the part of non-orthogonal bases \( (\phi^*) \), where the condition \( \text{GRAD} u, \text{GRAD}^*_W u \) is not fulfilled at the “predictor” stage (explicit time layer, known iteration, etc). For circuits with limited directwind, an appropriate set of cells \( (\Omega^*) \) is generated in the formation of which at least one basis of \( (\phi^*) \) is involved. Such locally regularized schemes in the sense of a sign-definiteness of the operator divgrad will not have strict properties of sign-definiteness and self-adjointness of this operator. However, from the point of view of physical applications, the preservation of the sign-definiteness of quadratic forms in the above sense is useful because it allows one to correctly approximate the exact square of the gradient of the thermodynamic quantities in the depression wells, in particular, the associated with it Joule–Thomson effect in the nonisothermal filtration processes considered below.

In the model of the filtration fluidodynamics with gas hydrate inclusions, the mechanism of contravariant directwind \( W_{\phi}(\lambda) \) is generated in the formation of which at least one basis of \( (\phi^*) \) is involved. Such locally regularized schemes in the sense of a sign-definiteness of the operator divgrad will not have strict properties of sign-definiteness and self-adjointness of this operator. However, from the point of view of physical applications, the preservation of the sign-definiteness of quadratic forms in the above sense is useful because it allows one to correctly approximate the exact square of the gradient of the thermodynamic quantities in the piezoelectroconducting part of the discrete connected task of nonisothermal filtration considered below.

According to the studies of [5], the absolute permeability \( k(S_{\nu}) \) in the bases \( \phi \) on the edges \( (\lambda(\phi)) \) forming these bases is always chosen downstream (i.e., downwind over by thawing). Relative permeabilities \( k_{\nu}(S_{\nu}) \) and \( k_{\nu}(1 \) \( -S_{\nu}) \), as a rule, are taken upstream (upwind by water and gas saturation), i.e. as in a two-phase melt zone with no hydrate. However, in accordance with the conditions analyzed in [5], a change in the sign of the directwind (i.e., downwind along the water and gas saturation) is also possible here.

4. Free-volume approximation of divergent-piezoelectric difference schemes for filtration fluid dynamics problems with gas hydrate inclusions

We introduce some notation for the grid functions of the support-operators method (section 3, see also figure 1). We will refer to its nodes previously presented in the continuum model quantities \( \{\pi, S_{\nu}, S_{\omega}, \rho_{\nu}, \rho_{\omega}, \rho_{g}, \rho_{s}, P, T, \varepsilon_{\nu}, \varepsilon_{w}, \varepsilon_{g}, \varepsilon_{s}, \mu_{\nu}, \mu_{g}, k_{\nu}, k_{g}, q_{w}, q_{g}, q_{s}\} \). To the grid bases \( \phi \) in accordance with section 3, we classify the vector functions \( V_{\nu}, V_{g}, \nabla P, \nabla T, W \).

We assign grid functions that represent the discontinuous material properties of substances to cells \( \Omega \): \( m, k, \nu_{\nu}, \nu_{w}, \nu_{g}, \lambda_{w} \).

The relations are obvious
\[ m_{\omega} = \sum_{\phi(\omega)} V_{\phi} m_{\Omega(\phi)}, \quad (1 - m_{\omega}) = \sum_{\phi(\omega)} V_{\phi}(1 - m_{\Omega(\phi)}) = V_{\nu} - m_{\omega}, \quad V_{\omega} = \sum_{\phi(\omega)} V_{\phi}, \quad (21) \]
i.e. \( \bar{m}_\omega \) and \( (1 - m)_\omega \) represent the volume of the pore domain \( d(\omega) \) (see figure 1) and its frame part, respectively.

Then on the temporary layers \( t \) and \( \hat{t} = t + \tau \) (\( \tau > 0 \) is the time step), we introduce the difference derivatives with respect to time and to interpolations in mesh nodes \( \omega \ a_t = (\hat{a} - a)/\tau \), 
\[
a^\delta = \delta a + (1 - \delta)a.
\]
Here the interpolation weight \( \delta \) may depend on the spatial grid node \( \omega \), the members with symbol \( \hat{\cdot} \) mean the members on the implicit layer over time.

Under the value
\[
d_\nu = \frac{\sqrt{(mS_\nu)}}{\sqrt{(mS_\nu)} + \sqrt{(mS_\nu)}}, \quad 0 < S_\nu < 1
\] we mean the free-volume time approximation of the grid functions given at the nodes \( \omega \), i.e. interpolation weight \( d_\nu \) is determined by the proportion of the pore volume, intended for free movement of the liquid and gas. The choice of such an approximation will allow us in the future to produce discrete transformations of equations related to their splitting by physical processes, close to continual ones. Other arbitrary interpolations with respect to time will be denoted by \( [] \). They can relate not only to grid nodes \( \omega \), but also to its other elements (bases \( \phi \) and etc).

Meaning the subscript \( S \) in vector analysis operations DIN\(_S\) and GRAD\(_S\) one of the types of contravariant directwind described above (or its absence) monotonizing the transfer by saturation \( S_w \) and \( S_\nu \), we write the approximation of equations (1), (2) and (5) in the following form.

Equations of continuity, representing the balance of the mass of the water and gas components are
\[
\{  m[S_\nu S_w \rho_w + (1 - S_\nu) \rho_\nu \beta_w] \}_{t} + \text{DIN}_s(\rho_w \mathbf{V}_w) + q_w = 0, \quad (23)
\]
\[
\{  m[S_\nu (1 - S_w) \rho_g + (1 - S_\nu) \rho_\nu (1 - \beta_w)] \}_{t} + \text{DIN}_s(\rho_g \mathbf{V}_g) + q_g = 0. \quad (24)
\]

With the help of the operator GRAD\(_s\), water flows \( (\rho_w \mathbf{V}_w) \) and gas \( (\rho_g \mathbf{V}_g) \) are approximated in grid bases \( \phi \) considering sampling Darcy’s law (3), (4), for example, on the implicit time layer by any of the standard methods \([7, 11]\).

\[
(\rho_w \mathbf{V}_w)^s_{\phi} = - \left( \rho_w \frac{k k_{rw}}{\mu_w} \right) \text{GRAD}_s \mathbf{P} + \left( \rho_w \frac{k k_{rw}}{\mu_w} \right) \frac{\nabla \mathbf{q}}{\Delta \phi}, \quad (25)
\]
\[
(\rho_g \mathbf{V}_g)^s_{\phi} = - \left( \rho_g \frac{k k_{rg}}{\mu_g} \right) \text{GRAD}_s \mathbf{P} + \left( \rho_g \frac{k k_{rg}}{\mu_g} \right) \frac{\nabla \mathbf{q}}{\Delta \phi}. \quad (26)
\]
Here \( ()^s \) means an approximation of the corresponding expressions \( () \) in grid bases \( \phi \) with some interpolation in time.

However, in the presence of a thermobaric dependence of the form (7) for preserving the continual properties of the sign-definiteness of the quadratic forms of the gradients of thermodynamic quantities of the form \( \int \varepsilon \nabla \cdot (\mathbf{P} \mathbf{V}) \, dV \) (as equation (37) below), the form of the Darcy’s law in the energy formulation is more preferable. We obtain it from the following considerations.

Taking into account the thermobaric dependence (7) in the three-phase equilibrium zone, hydrate-water-gas can be
\[
d\varepsilon_w = \varepsilon^{\prime}_{wp} dP, \quad d\varepsilon_g = \varepsilon^{\prime}_{rg} dP.
\]
Where \( \varepsilon^{\prime}_{wp} \) and \( \varepsilon^{\prime}_{rg} \) are the total derivatives of the internal energy with respect to pressure, taking into account (7). Then the Darcy’s law (3), (4) in the grid bases (formed by the nodes in which the thermobaric relation (7) is satisfied) can be represented in the energy form:
\[
(\rho_w \mathbf{V}_w)^s_{\phi} = - \left( \rho_w \frac{k k_{rw}}{\mu_w \varepsilon^{\prime}_{wp}} \right) \text{GRAD}_s \varepsilon^s_{w}(\delta_\nu) + \left( \rho_w \frac{k k_{rw}}{\mu_w} \right) \frac{\nabla \mathbf{q}}{\Delta \phi}, \quad (27)
\]
\[(\rho_g \mathbf{V}_g)_{\phi}^\epsilon = - \left( \frac{\rho_g}{\mu_g \mathbf{e}_{\phi}} \right)^\epsilon \text{GRAD}_s (\delta) + \left( \frac{\rho_g}{\mu_g} \right)^\epsilon g \mathbf{k}. \] (28)

In this way
\[
(\rho_w \mathbf{V}_w)_{\phi} = - \left\{ (\rho_w \mathbf{V}_w)_{\phi}^\epsilon \right\},
\]
\[
(\rho_g \mathbf{V}_g)_{\phi} = - \left\{ (\rho_g \mathbf{V}_g)_{\phi}^\epsilon \right\}.
\]

The equation for the balance of internal energy approximating (5) has the form:
\[
\left\{ \mathcal{M}(S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \delta) + (1 - S_w) \rho_v \varepsilon_v + (1 - \mathcal{M}) \rho_s \delta \right\}_t + \mathcal{D}_w \left[ (\varepsilon_w)_{up} (\rho_w \mathbf{V}_w) - \mathcal{D}_g \left[ (\varepsilon_g)_{up} (\rho_g \mathbf{V}_g) \right] \right] + \mathcal{D}_w \left\{ (\mathbf{P} (\mathbf{V}_w + \mathbf{V}_g)) \right\} + \mathcal{D}_w \mathbf{W} - q - \delta = 0.
\]

Index up in the expression for the energy of water \((\varepsilon_w)_{up}\) indicates that the respective values are taken up (upwind) by the water flow \((\rho_w \mathbf{V}_w)\) in a previously defined divergence \(\mathcal{D}_w(\rho_w \mathbf{V}_w)\). Similarly, the index up is understood in the expression for the energy of the gas \((\varepsilon_g)_{up}\).

Work of pressure forces \(\mathbf{P} (\mathbf{V}_w + \mathbf{V}_g)\) and the total heat flux \(\mathbf{W} \) in the medium are approximated in grid bases \(\phi\), for example, on the implicit time layer standard manner [7, 11]:
\[
[\mathbf{P} (\mathbf{V}_w + \mathbf{V}_g)]_{\phi} = \left( \frac{P}{\rho_w} \right)_{\phi} (\rho_w \mathbf{V}_w)_{\phi}^\epsilon + \left( \frac{P}{\rho_g} \right)_{\phi} (\rho_g \mathbf{V}_g)_{\phi}^\epsilon.
\]

Further, the discrete analogue of the piezoconductive equation (14)–(18) physically split with the saturation block (23), (24), but difference-equivalent to the system of first principles of the model (23), (24), (31) has the form:
\[
\delta_{\epsilon} \left\{ \left[ \mathcal{M} S_v \right] (1 - \delta) \right\} \frac{\rho_w (\varepsilon_v)}{\rho_w (\delta_v)} + \left[ \mathcal{M} (1 - S_w) \right] (1 - \delta) \right\} \frac{\rho_g (\varepsilon_g)}{\rho_g (\delta_g)} + \left[ \mathcal{M} \right] (1 - \delta) \right\} \frac{\rho_s (\varepsilon_s)}{\rho_s (\delta_s)}
\]
\[
+ \left[ \psi / (\rho_m \nu) \right] \left\{ \left[ \mathcal{M} S_v \right] S_w \rho_w (1 - \delta) \right\} (\varepsilon_v)_{up} + \left[ \mathcal{M} (1 - S_w) \rho_g (1 - \delta) \right\} (\varepsilon_g)_{up} + \left[ (1 - \mathcal{M}) \rho_s \varepsilon_s \right] + \delta_{\epsilon} \mathcal{D}_g - \left[ \psi / (\rho_m \nu) \right] \left[ \mathcal{D}_g \right] - \delta = 0,
\]
\[
\delta_{\epsilon} = \left[ \beta_w \varepsilon_w + (1 - \beta_w) \varepsilon_g \right] - \varepsilon_v, \]
\[
\left[ \psi / (\rho_m \nu) \right] = \left[ \beta_w / (\rho_w) (\delta_v) + (1 - \beta_w) / (\rho_g) (\delta_g) \right] - 1 / (\rho_s) (\delta_s),
\]
\[
\mathcal{D}_g = \mathcal{D}_w (\rho_w \mathbf{V}_w) / (\rho_w) (\delta_v) + \mathcal{D}_w (\rho_g \mathbf{V}_g) / (\rho_g) (\delta_g),
\]
\[
\mathcal{D}_g = \mathcal{D}_w (\varepsilon_w)_{up} (\rho_w \mathbf{V}_w) - (\varepsilon_v) (\delta_v) \mathcal{D}_w (\rho_w \mathbf{V}_w)
\]
\[
+ \mathcal{D}_w (\varepsilon_g)_{up} (\rho_g \mathbf{V}_g) - (\varepsilon_g) (\delta_g) \mathcal{D}_w (\rho_g \mathbf{V}_g) + \mathcal{D}_w \left\{ (\mathbf{P} (\mathbf{V}_w + \mathbf{V}_g)) \right\} + \mathcal{D}_w \mathbf{W} - (q - \varepsilon_w) \left\{ \mathcal{D}_w \right\} + \varepsilon_g \left\{ \mathcal{D}_w \right\}.
\]

In the expression \(\mathcal{D}_g\), which appears in (33), there is a monotonic (upstream) energy approximation for \(\varepsilon_w(\delta_v)\) and \(\varepsilon_g(\delta_g)\) in the corresponding combinations of divergent expressions containing these quantities.
5. Results of calculations

In order to compare schemes with free-volume approximation (23)–(26), (33) with incompletely conservative difference schemes approximating a piezoconductive medium with gas hydrate inclusions, we consider the computational experiment given in this section. As an example of a scheme with an incompletely conservative approximation, i.e. not reducible to the divergent difference analog of equations (1)–(7), we choose the well-known IMPIS method [12]. These schemes are implicit in pressure and saturation. The construction and testing of the IMPES scheme splitting by physical processes, implicit in thermodynamics (pressure, temperature) and explicit on saturations (water saturation, thawing) with reference to the modeling of fluid dynamic processes with hydrate inclusions are described in detail in [6]. In the scheme with free-volume approximation (23)–(26), (33), the approximation in time of terms not related to nonlinear interpolation with weight \( \delta_\nu \) (22), in this test is selected the same as in IMPIS method, adapted to the calculation of processes with hydrate inclusions, i.e. implicit in saturations \((S_w, S_g)\) and thermodynamic variables \((P, T)\). These terms in the scheme with free-volume approximation are marked by a “wave”.

Internal energies of skeletal, water and gas phases in the model are taken proportional to the temperature [13]: \( \varepsilon_l = \varepsilon(T, l = s, w, g) \). Here \( \varepsilon_s, \varepsilon_w, \varepsilon_g \) are appropriate specific heats of skeletal, water and gas. Internal energy of hydrate \( \varepsilon_w \) is calculated according to (9) with allowance for (12). Gas in the following test is considered ideal, also adiabatic cooling effect associated with the selection of the gas collecting zone is absent. In this approximation, at the boundaries of the source range (selection of gas proportional to differential pressure) saturations peaks arise, which are associated with the skin dissipation of pressure inside the gas sampling region at these boundaries. The effect is described by the piezoconductive process of gas hydrates and studied in detail in [6]. We choose these singular singularities of the solution (the peaks of the thawing and water saturation) on the inner boundaries of the zone of sharp depression in the reservoir for comparison schemes with free-volume approximation and IMPIS-schemes.

So, consider the following spatial one-dimensional process in the interval \( x \in [0, l] \), \( l \) is the length of the calculated area. In it at the initial instant of time, the pressure \( P(x, 0) = 2 \times 10^5 \) Pa, water saturation \( S_w(x, 0) = S_{w}^* \) and thawing \( S_g(x, 0) = S_{g}^* \) are homogeneous in space, \( 0 < S_{w}^* < 1 \) and \( 0 < S_{g}^* < 1 \) are constant values. It is considered that the share of thermal conductivity in the overall heat transfer balance is negligible compared to convection, i.e. in the energy equation, the conductive component is assumed to be equal to zero \((\nabla \cdot \mathbf{W} = 0)\). Acceleration of free fall is also not taken into account \((g = 0)\). The boundaries of the design area are assumed to be impermeable solid “walls”, i.e. the flow through them is zero:

\[
V_w|_{x=0} = 0, \quad V_g|_{x=0} = 0, \quad V_w|_{x=l} = 0, \quad V_g|_{x=l} = 0, \quad t > 0.
\]

Suppose that in a narrow spatial domain the source works:

\[
q_w = \alpha(P - P^*), \quad q_g = \beta(P - P^*), \quad q_\varepsilon = \varepsilon_w q_w + \varepsilon_g q_g,
\]

where \( P^* \) is a constant value, \( \alpha \) and \( \beta \) are characteristics of the source (drain) in the bottomhole zone, caused by the pressure difference inside the well and in the formation. Everywhere in the future we will assume \( \alpha = 0, \beta = 0.00001 \) s/m². In this case the dimension of the pressure \([P] = \)Pa. The source is valid only in the spatial domain \( x \in [0.4, 0.6] \) m.

To calculate the following parameter values were selected characteristic Messoyakhskoye gas hydrate deposits [14–16]:

\[
\rho_w = 10^5 \text{ kg/m}^3, \quad \rho_\nu = 910 \text{ kg/m}^3, \quad \rho_s = 2800 \text{ kg/m}^3, \quad 
\beta_w = 0.9, \quad m = 0.35, \quad A = 7.28, \quad B = 169.7 \text{ K}.
\]

Here, approximation [17] is selected as thermobaric depending \( T_{\text{dis}} = f(P) \), see (7):

\[
T = A \ln P + B \text{ at } [P] = \text{Pa}.
\]
Figure 2. Distribution of thawing for moments of time 1, 10, 30 s. Free-volume approximation.

Further $\mu_w = 10^{-3}$ Pa s, $\mu_g = 0.014 \times 10^{-3}$ Pa s, $c_w = 4165$ J/(kg K), $c_g = 2500$ J/(kg K), $c_s = 873$ J/(kg K), $M = 0.016$ kg/mol, $h = 514810$ J/kg, $R = 8.31$ J/(mol K), $S_w^* = 0.6$, $S_g^* = 0.5$, $k(S_w) = k_0(S_w)^3$, $k_0 = 10$ mD = $10^{-14}$ m$^2$, $P^* = 2$ MPa;

$$k_{tw}(S_w) = 1.477S_w^5 - 1.587S_w^6 + 1.11S_w^7 - 0.0473,$$
$$k_{tg}(S_w) = 1.044 - 1.7S_w + 0.6S_w^2.$$ 

The minimum value of water saturation $S_{min} = 0.55$;

$$k_{tw}(S_w) = 0, \quad k_{tg}(S_w) = k_{tg}(S_{wmin}) \text{ at } S_w \leq S_{wmin}.$$ 

The maximum value of water saturation $S_{max} = 0.9$;

$$k_{tw}(S_w) = k_{tw}(S_{wmax}), \quad k_{tg}(S_w) = 0 \text{ at } S_w \geq S_{wmax}.$$ 

The length of the model pipe is assumed to be equal to $l = 1$ m, a step in the space coordinate $h = 0.01$ m. Calculations are given for time $t = 1, 10, 30$ s. In figures 2–5 show the results of calculations using the free-volume approximation scheme.

The distributions of thawing, water saturation, pressure and temperature for the moments of time 1, 10 and 30 s, respectively, calculated by the scheme with free-volume approximation, are shown in figures 2–5. The solutions for thawing obtained by different methods (IMPIS-scheme and free-volume approximation) calculated on the same grid ($h = 0.01$ m) with the same time step ($dt = 0.00753$ s) were compared with the exact solution. The limit solution, taken as a half-sum calculations by IMPIS-scheme and by the free-volume approximation was used as the accurate solution (grid pitch is reduced to $h = 1/16000$ m). At moment of time $t = 10$ s calculation the difference between the calculations with free-volume approximation and the exact solution in the L2-norm was 0.00006234, between calculations on the IMPIS-scheme and the exact solution—0.00005998, respectively.
Figure 3. Distribution of water saturation for moments of time $t = 1, 10 \text{ and } 30$ s. Free-volume approximation.

Figure 4. Distribution of pressure for moments of time 1, 10, 30 s. Free-volume approximation.
Figure 5. Distribution of temperature for moments of time $t = 1, 10$ and $30$ s. Free-volume approximation.

Figure 6. Distribution of thawing at the moment of time $t = 10$ s. Free-volume approximation (dotted line), IMPIS-scheme (dot dash) and the exact solution (solid line).
Figure 7. Distribution of thawing at the moment of time $t = 10$ s. IMPIS-scheme (dot dash) and the exact solution (solid line).

Figure 8. Distribution of thawing at the moment of time $t = 10$ s. Free-volume approximation (dotted line) and the exact solution (solid line).
Calculations of the spatial distributions of the thawing at moment of time \( t = 10 \) s according to the IMPIS scheme and the scheme with free-volume approximation along with the exact solution are shown in figure 6. The relative accuracy of iterative convergence in the experiments was 1%. Separately comparing the exact solution with each of the methods is also presented in figures 7 and 8. The water saturation, pressure and temperature in calculations with the free-volume approximation scheme and the IMPIS scheme are practically the same.

We see that the solutions obtained by both methods are insignificantly different. Their difference from the exact solution is noticeable in the singularity zones. In this case, the solution obtained by the free-volume method accurately satisfies the equation for the balance of internal energy in the form (31). We also note that interpolation with weight \( \delta_{\nu} \), see (22), where it is introduced, has a second order in time.

6. Conclusion

In this paper, a family of discrete algorithms splitted by physical processes with free-volume approximation of the piezoconductive equation in a medium with hydrate inclusions was constructed on the grids of the theory of the support operators method applied to the processes of a two-component three-phase filtration fluid dynamics with gas hydrate inclusions. These algorithms allow making applied calculations with a large step in time as well as reducing the dimensionality of solved algebraic problems and these are difference-equivalent to the system of the first balanced principles of the model. Calculations based on the proposed approach are presented. Also, in the context of the specifics of saturation transfer processes in a filtration medium with hydrate inclusions, various methods of the direct wind approximation of these processes are considered, along with simultaneous preservation of the properties of sign-definiteness and self-adjointness of differential divergence–gradient operators connected with the velocity field providing this transfer. This allows qualitatively approximate the gradient changes in thermodynamic quantities in the depression wells, the Joule–Thomson effect, and other physical processes inherent in the theory of nonisothermal filtration.

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