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## A NUMERICAL APPROACH TO STUDY THE THERMAL INFLUENCE ON GAS HYDRATES BY PHYSICAL PROCESS SPLITTING

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Abstract. The method of numerical simulation based on the splitting by physical processes of gashydrodynamic processes, which occur during the dissociation of gas hydrates in a porous medium, is described. In this paper, a coupled discrete model of a two-component  $(H_2O, CH_4)$  three-phase (water, methane, hydrate) filtration fluid dynamics and two-phase processes in a thawed zone with absence of gas hydrates in thermodynamic equilibrium has been developed, by using the splitting by physical processes as a valid assumption. The obtained split model is differentially equivalent to the discrete initial balance equations of the system (conservation of the mass components of the fluids and the total energy of the system), written in divergent form. Such an approach to create completely conservative difference schemes in the studied fluid-hydrate medium requires the introduction of a special free-volume nonlinear approximation of grid functions over time, which depends on the volume fraction in the pores occupied by fluids, and is simple to implement. The direct unsplit use of the studied system for the purposes of determining the dynamics of variables and constructing the implicit difference scheme required for calculations of filtering processes with large time steps is difficult. The paper also presents the method of coupled solutions of systems of equations describing the processes in various fields, each of which is characterized by its own set of coexisting phases, and the coordination of computational schemes for them is not an automatic process. In the results of the calculations, the volumetric three-phase phase transitions were numerically investigated using a single calculation with a variable number of phases region of the entire plane of the P and T parameters. Using the example of the Messoyakha's gas hydrate deposit, the local processes of technogenic depressive impact directly near the wells on the dynamics of the gas distribution of gas hydrates thawing and formation of thawed two-phase zones were studied.

**Key words.** Gas hydrates, filtration, thawed zone, support operators, and completely conservative difference schemes.

#### 1. Introduction

One of the risks arising from the exploration of hydrocarbon deposit in northern areas is a possibility of sudden gas blowout. Such blowouts can be connected with gas hydrates decomposition as a result of technogeneous impact during drilling and exploitation of wells [1] and lead to crashes and environmental incidents especially in case of sea reservoirs.

Mathematical simulation of the gas-hydrodynamic processes during dissociation of gas hydrates in porous medium is an important part of the complex analysis of the problem. The modeling consists of calculation of the pressure field, water and hydrate saturation fields, and investigating the conditions leading to undesirable effects. Whole research should include a joint study of heat transfer, fluid dynamics and stress-strain state of the rocks in the investigated area. For the estimation of the impact of every single factor on the whole process, it is necessary to investigate each of them separately.

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In order to solve a wider class of problems, it is necessary to use numerical methods. As a base for mathematical modeling of the underground fluid dynamics with respect to gas hydrates dissociation, the equations of mass, momentum and energy balance are derived assuming that the processes are in thermodynamic equilibrium. This is compliant with the time scale typical to the reservoirs exploration. The filtration area is naturally divided into two zones: the three-phase zone with gas, water and hydrate and thawed zone – without hydrates. Each zone has its own system of partial differential equations describing fluid motion. So it is necessary to sew them together in the whole (P - pressure, T - temperature) area to unified numerical scheme. This is achieved by studying the analytical conditions for the consistency of the equation systems with help of the method of characteristics.

In the proposed approach, in the three-phase zone, the initial system of equations is transformed into a two-block mathematical model describing a multicomponent flow in a porous medium, taking into account the dissociation of gas hydrates with splitting by physical processes. The model includes a block with a system of hyperbolic equations for water saturation and thaw on the background of fixed filtration rates, and a block containing the piezoconductivity equation for determining the pressure in the reservoir with gas hydrate inclusions.

In the gas-water-hydrate thermodynamic equilibrium zone, the pressure and temperature are related by well-studied dependencies, for which one of several approximations is usually chosen [2]. In this paper, T = AlnP + B was used as the approximation, where A and B are the empiric coefficients.

The initial boundary value problem is solved using the finite difference method. In constructing schemes, an upwind approximation is used for water saturations and a downwind approximation is used for thaw. This technique follows from the analysis of the hyperbolicity of the system of equations against the background of a fixed velocity field determined by Darcy's law (see subsection 2.3).

The use of splitting by physical processes allows us to use an explicit-implicit scheme, to use rather large time steps; it sharply increases the counting rate, which makes it possible to carry out a number of calculations with various parameters and compare the results.

In this work, a special technique is used to combine the calculations of a threephase zone containing gas, water and hydrate, and thawed zone, with the absence of gas hydrates, into one calculation scheme (see subsection 5.6).

For more complex calculations that take into account non-one-dimensionality, we can use an approach to numerical simulation based on the method of support operators, those application to filtering problems was started in [3, 4]. This method, based on the use of irregular grids, makes it possible to approximate regions of complex geological and lithological structure, to take into account the different scales of heterogeneities within a one difference scheme (from the near-well zone to the size of the reservoir and even the region). In this paper it is expanded in the case of filtration processes involving gas hydrates. In accordance with the proposed algorithm for the splitting of the equilibrium model by physical processes, in the thawed zone and in a medium with gas hydrate inclusions, a joint family of twolayer completely conservative difference schemes of the support operators method with spaced time scales has been constructed.

In the future, the function  $S_{\nu}$  we will denote the volume fraction in the pores attributable to free water and gas in the hydrate-saturated part of the porous medium. The function  $S_w$  we will denote water saturation.

On the irregular metric grids of the theory of the support operators method as applied to the specificity of the transfer processes of saturation and internal energy of water and gas in a hydrated medium the methods of approximating the relative and absolute permeabilities of the medium corresponding to these processes were considered, while simultaneously maintaining continuum properties divgrad operations in their difference form related to the velocity field that provides this transfer. This is connected with another computational problem of modeling the filtration fluid dynamics of a hydrated medium, which consists in the need to approximate the squares of thermodynamic variables (internal energies or pressures of free water and gas) near depressed well craters with singular features. Such gradient quadratic forms are found in the discrete equation of the piezoconductivity of filtration fluid dynamics of a hydrated medium studied in this work and determine the dynamics of a nonlinear, quadratic in the gradient the transfer of thermodynamic parameters of the medium. It is possible to ensure positive definiteness of such quadratic forms by invoking the theory of metric grids of the support operators method, but only with preservation of the continual properties of *divgrad* operations in their difference form related to the field of the velocities determining this nonlinear transfer. Monotonization of the transfer of saturation processes by functions  $S_{\nu}, S_{w}$ , when used in the classical form, violates the properties of selfadjointness and sign-definiteness of these discrete vector analysis operations. In this work, we use the mechanism of monotonization of the grid solution which simultaneously ensures effective monotonization of the approximation on  $S_{\nu}, S_w$  to nonlinear transfer of the internal energies of free water and gas and preservation of the sign-definiteness of the quadratic gradient values of thermodynamic quantities in the hydrated piezoconductive part of the problem.

Filtration fluid dynamics of free water and gas in the presence of solid hydrate inclusions in a porous medium has a number of specific features.

First of all, according to the rule of the Gibbs phase, such a thermodynamic equilibrium two-component  $(H_2O, CH_4)$  three-phase (hydrate and free water and gas) system has only one thermodynamic degree of freedom. That is, there is a thermobaric connection  $T_{dis} = f(P)$  between the dissociation temperature of the gas hydrate and pressure. It is clear that in this situation any of them can be chosen as the main thermodynamic variable (for example, the internal energies of water or gas), if through them the temperature and pressure are expressed. In the future we will need this in order to present the fluid dynamics of a hydrated medium by Darcy laws in a discrete energy formulation (see 4). However, it must be borne in mind that in calculations in the thawed hydrated zone in the medium there are two independent thermodynamic parameters (P, T).

In the results of the calculations, the region of three-phase volume phase transitions was numerically investigated with a single calculation with a variable number of phases in the entire plane of the P and T parameters. Using the example of the Messoyakha's gas hydrate deposit, local processes of technogenic depressive effects directly near the wells on the dynamics of the spatial distributions of gas hydrates thaw and the formation of thawed two-phase zones were studied. Also on the tetrahedral grids in a spatially three-dimensional case, model calculations of piezoconductive processes in a three-phase medium with hydrated solid-phase inclusions near the depression wells are presented.

## 2. Formulation of the problem

**2.1.** Three-phase medium with hydrate inclusions. In the spatial domain O with the boundary  $\partial O$ , we consider the thermodynamic equilibrium two-component (water, methane) three-phase equations of filtration fluid dynamics with gas hydrate inclusions:

(1) 
$$\frac{\partial}{\partial t} \left\{ m \left[ S_{\nu} S_{w} \rho_{w} + (1 - S_{\nu}) \rho_{\nu} \beta_{w} \right] \right\} + div \left( \rho_{w} \mathbf{V}_{w} \right) + q_{w} = 0,$$

(2) 
$$\frac{\partial}{\partial t} \left\{ m \left[ S_{\nu} (1 - S_{w}) \rho_{g} + (1 - S_{\nu}) \rho_{\nu} (1 - \beta_{w}) \right] \right\} + div \left( \rho_{g} \mathbf{V}_{g} \right) + q_{g} = 0,$$

(3) 
$$\mathbf{V}_w = -\frac{\kappa \kappa_{rw}}{\mu_w} (\nabla P - g\rho_w \mathbf{k}),$$

(4) 
$$\mathbf{V}_g = -\frac{kk_{rg}}{\mu_g} (\nabla P - g\rho_g \mathbf{k}),$$

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(5) 
$$\frac{\partial}{\partial t} \left\{ m \left[ S_{\nu} (S_{w} \rho_{w} \varepsilon_{w} + (1 - S_{w}) \rho_{g} \varepsilon_{g}) + (1 - S_{\nu}) \rho_{\nu} \varepsilon_{\nu} \right] + (1 - m) \rho_{s} \varepsilon_{s} \right\} \\ + div \left\{ \rho_{w} \varepsilon_{w} \mathbf{V}_{w} + \rho_{g} \varepsilon_{g} \mathbf{V}_{g} + \left[ P(\mathbf{V}_{w} + \mathbf{V}_{g}) \right] \right\} + div \mathbf{W} + q_{\varepsilon} = 0,$$

(6) 
$$\mathbf{W} = -\{m[S_{\nu}(S_{w}\lambda_{w} + (1 - S_{w})\lambda_{g}) + (1 - S_{\nu})\lambda_{\nu}] + (1 - m)\lambda_{s}\}\nabla T, (7) 
$$T_{dis} = f(P)$$$$

(with some boundary conditions) with the integral relation:

(8) 
$$\int_{O} (\mathbf{X}\nabla u) dV + \int_{O} u \, div \, \mathbf{X} dV = \int_{\partial O} u(\mathbf{X}, d\mathbf{s})$$

The indices  $l = g, w, \nu, s$  refer to gas, water, hydrate, skeleton of porous medium. Here (1) is the balance equation of the water mass, (2) is the balance equation of the methane mass, (3) is Darcy's law, which determines the velocity of free water  $\mathbf{V}_w$  in the pores of a two-component immiscible system (water, methane) with the absolute permeability  $\mathbf{k} = k(\mathbf{r}, S_{\nu}, P)$  and the relative permeability  $k_{rw} = k_{rw}(S_w)$ .  $\mu_w$  is the viscosity of water. The equation (4) is understood in a similar way as Darcy's law for the free methane velocity  $\mathbf{V}_{g}$  with the relative permeability  $k_{rq} = k_{rq}(S_w)$  and the viscosity  $\mu_q$ . Finally, (5) is the balance equation for the total internal energy of the system, including the energies of free water, free methane, hydrate, and skeleton.  $\varepsilon_l$  are understood as the internal energies of components mass units. The equation (6) determines the total heat flow **W** in a medium with the thermal conductivity  $\lambda_l(P,T)$ .  $g\mathbf{k}$  is the gravitational acceleration, which is directed vertically down; P is the pressure;  $S_w$  is the water saturation,  $\nu$  is the hydrate saturation;  $S_{\nu} = 1 - \nu$  is the hydrate thaw;  $\rho_l(P,T)$  are the densities of the phases;  $\beta_w$  is the mass fraction of water in hydrate; r is the radius vector; t is time;  $q_w, q_g$  and  $q_{\varepsilon}$  are the corresponding source densities, which are dependent on the parameters  $(t, \mathbf{r}, S_w, S_\nu, P, T)$ . According to the Gibbs phase, the three-phase two-component hydration system is multivariate, i.e. has one degree of freedom (temperature or pressure) [10]. Hence, the dependence (7) is unambiguous for a gas hydrate that is in equilibrium with liquid water or ice.  $u, \mathbf{X}$  in (8) are the arbitrary scalar (temperature, pressure, internal energy, etc.) and the arbitrary vector which is physically related to the gradient flow of this scalar quantity.

The enthalpies of the unit mass  $i_l = \varepsilon_l + P/\rho_l$  of hydrate, free water, and gas are thermodynamically consistent in the following relationship:

(9) 
$$\beta_w i_w + (1 - \beta_w) i_g = i_\nu + h,$$

where h is the latent heat of a phase transition of a hydrate unit mass. The following equation is also suitable [11] for the specific (per unit mass) enthalpies of phases:

(10) 
$$di_l = c_{pl}(-k_{dl}dP + dT)$$

with the throttling coefficients

(11) 
$$k_{dl} = \frac{1}{c_{pl}} \left[ T \left( \frac{\partial V_l}{\partial T} \right)_p - V_l \right].$$

Here the index "p" at the parentheses means that the partial derivative with respect to temperature is taken at constant pressure;  $c_{pl}$  and  $V_l = 1/\rho_l$  are the specific heat capacities (at constant pressure) and the phase volumes. In particular, for the gas phase with the following equation of state:

(12) 
$$\rho_g = \frac{P}{z_g R T},$$

the throttling coefficients holds true

(13) 
$$k_{dg} = \frac{RT^2}{c_{pg}P} \frac{\partial z_g}{\partial T},$$

which means the presence of the Joule-Thomson effect  $(k_{dg} \neq 0)$  for a nonideal gas with a coefficient of supercompressibility  $z_g$  in the studied processes of nonisothermal filtration.

We exclude  $S_w$  and  $S_{\nu}$  functions from the time derivative of equations (1), (2), (5) and obtain the piezoconductivity equation for fluid dynamics with hydrate inclusions in the following form:

$$m\delta_{\varepsilon} \left\{ S_{\nu} \left[ S_{w} \frac{1}{\rho_{w}} \frac{\partial \rho_{w}}{\partial t} + (1 - S_{w}) \frac{1}{\rho_{g}} \frac{\partial \rho_{g}}{\partial t} \right] + (1 - S_{\nu}) \frac{1}{\rho_{\nu}} \frac{\partial \rho_{\nu}}{\partial t} + \frac{1}{m} \frac{\partial m}{\partial t} \right\}$$

$$+ \frac{\psi}{m\rho_{\nu}} \left\{ m \left\{ S_{\nu} \left[ S_{w} \rho_{w} \frac{\partial \varepsilon_{w}}{\partial t} + (1 - S_{w}) \rho_{g} \frac{\partial \varepsilon_{g}}{\partial t} \right] + (1 - S_{\nu}) \rho_{\nu} \frac{\partial \varepsilon_{\nu}}{\partial t} \right\}$$

$$+ \frac{\partial [(1 - m) \rho_{s} \varepsilon_{s}]}{\partial t} \right\} + \delta_{\varepsilon} DIG + \frac{\psi}{m\rho_{\nu}} DIG_{\varepsilon} = 0.$$

Here

=

$$DIG = \frac{1}{\rho_w} div(\rho_w \mathbf{V}_w) + \frac{1}{\rho_g} div(\rho_g \mathbf{V}_g) + \frac{q_w}{\rho_w} + \frac{q_g}{\rho_g},$$
  

$$DIG_{\varepsilon} = [\operatorname{div}(\rho_w \varepsilon_w \mathbf{V}_w) - \varepsilon_w div(\rho_w \mathbf{V}_w)] + [\operatorname{div}(\rho_g \varepsilon_g \mathbf{V}_g) - \varepsilon_g \operatorname{div}(\rho_g \mathbf{V}_g)] + div[P(\mathbf{V}_w + \mathbf{V}_g)] + \operatorname{div}\mathbf{W} + (q_{\varepsilon} - \varepsilon_w q_w - \varepsilon_g q_g),$$
  

$$= \rho_w \mathbf{V}_w \nabla \varepsilon_w + \rho_g \mathbf{V}_g \nabla \varepsilon_g + \operatorname{div}[P(\mathbf{V}_w + \mathbf{V}_g)] + \operatorname{div}\mathbf{W} + (q_{\varepsilon} - \varepsilon_w q_w - \varepsilon_g q_g).$$
  
And  

$$\frac{q_w}{\rho_w} = \frac{1}{\rho_w} \frac{\rho_w}{\rho_w} \frac{1}{\rho_w} \frac{\rho_w}{\rho_w} \frac{1}{\rho_g} \frac{\rho_w}{\rho_w} \frac{1}{\rho_g} \frac{\rho_w}{\rho_w} \frac{1}{\rho_w} \frac{1}{\rho_w} \frac{\rho_w}{\rho_w} \frac{1}{\rho_w} \frac{1$$

$$\frac{\psi}{m\rho_{\nu}} = (\varphi - \frac{1}{\rho_{\nu}}) \ge 0, \ \varphi = \frac{\beta_w}{\rho_w} + \frac{(1 - \beta_w)}{\rho_g}$$
$$\delta_{\varepsilon} = \beta_w \varepsilon_w + (1 - \beta_w) \varepsilon_g - \varepsilon_v \ge 0,$$

are specific jumps (per unit mass) at the phase transition of the volume and internal energy, respectively.

We also use the notation:  $()_p = \frac{\partial}{\partial P}$ .

The equation (14) is the main piezoconductive-dissipative thermodynamic equilibrium equation of three-phase two-component fluid dynamics with hydrate inclusions. This equation is split with the block (1), (2), (3), (4) of saturation processes transfer. This block has mainly hyperbolic properties against the background of the thermodynamic parameters of the medium. We introduce a new value  $D_P$ . It is the pressure coefficient of the hydrate system:

(15)  
$$D_{p} = m\delta_{\varepsilon} \{S_{\nu}[S_{w}\frac{(\rho_{w})_{p}}{\rho_{w}} + (1 - S_{w})\frac{(\rho_{g})_{p}}{\rho_{g}}] + (1 - S_{\nu})\frac{(\rho_{\nu})_{p}}{\rho_{\nu}} + \frac{(m)_{p}}{m}\} + \frac{\psi}{m\rho_{\nu}} \{m\{S_{\nu}[S_{w}\rho_{w}(\varepsilon_{w})_{p} + (1 - S_{w})\rho_{g}(\varepsilon_{g})_{p}] + (1 - S_{\nu})\rho_{\nu}(\varepsilon_{\nu})_{p}\} + [(1 - m)\rho_{s}\varepsilon_{s}]_{p}\}.$$

We rewrite equation (14) in a more compact form

(16) 
$$D_P \frac{\partial P}{\partial t} + \delta_{\varepsilon} DIG + \frac{\psi}{m\rho_{\nu}} DIG_{\varepsilon} = 0.$$

The total pressure derivative is taken in (15) with respect to dependency (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), we obtain the equation (14) in the energy representation.

The physics of the piezoconductivity equation (14), (16) lies in its material coefficients  $(\delta_{\varepsilon}, \psi/m\rho_{\nu}, D_P)$ . Note also that the terms associated with a free non-ideal gas (g) in the non-stationary part of the piezoconductivity equation (14) and the gradient quadratic forms of thermodynamic quantities in the terms corresponding to gas in  $DIG_{\varepsilon}$  determine the Joule-Thompson effect in the medium under study [12]. The piezoconductivity equation (14) does not contain time derivatives of saturations  $(S_{\nu}, S_w)$  and in this sense is split with a block of saturation transport equations (1), (2). For fixed saturation values, the absence of capillary and gravitational terms (14) is a parabolic equation for pressure (or other thermodynamic value), if we consider one thermodynamic degree of freedom of the system (T = T(P)) in the sense of the Gibbs phase rule. However, in the piezoconductivity equation (14) there are terms of the gradient quadratic transfer of the form  $\rho \mathbf{V} \nabla \varepsilon$  for free water and gas in accordance with the Darcy laws (3), (4). At the discrete level, it is important to ensure the positivity of the approximation of the squares of the gradients of their thermodynamic quantities in the integral sense  $(\int_{\Omega} \rho \nabla \nabla \varepsilon dV)$ , in particular, this is due to the modeling of depression funnels near the wells. Upwind approximation of expressions  $\rho \mathbf{V} \nabla \varepsilon$  is necessary to monotonize a difference solution, understood as the process of energy transfer. Moreover, the approximation of the Darcy laws (3), (4) in simple cases should also satisfy upwind conditions for saturation  $S_w$  and downwind conditions for thawing  $S_{\nu}$ . Upwind approximation is understood in the same way as upstream waiting to calculate the phase mobility [5]. It is one of the possible methods for suppressing computational instability in simulating the transfer processes of any nature and is understood by us as monotonization (that is, the absence of oscillations) of a difference solution. Its meaning is reduced to the fact that, for computational stability, the invariants of the hyperbolic system of transport equations (or their approximations) are carried along the corresponding characteristics, and not towards them. If this drift coincides with the direction of the physical movement of the substance, then such an approximation is called upwind. It should be noted that in a hyperbolic system of equations describing the transfer process, its invariants can be transferred by characteristics not from the direction of the physical movement of a substance

(upwind), but from the opposite (downwind). This case takes place in the approximation of the thawing and is considered in subsection 2.3. The tools of the support operator method for the simultaneous discrete implementation of the above requirements (positive definiteness of quadratic forms, monotonization of difference solutions with respect to saturations  $(S_{\nu}, S_w)$  and energies  $(\varepsilon_w, \varepsilon_g)$ ) on irregular grids are considered in section 3.

**2.2. Two-phase thawed zone.** Similarly to subsection 2.1, we assume the thawing is  $S_{\nu} = 1$  and obtain a two-phase equation in the thawed zone,

(17) 
$$\frac{\partial}{\partial t} \{mS_w \rho_w\} + div \left(\rho_w \mathbf{V}_w\right) + q_w = 0$$

(18) 
$$\frac{\partial}{\partial t} \left\{ m(1-S_w)\rho_g \right\} + div \left(\rho_g \mathbf{V}_g\right) + q_g = 0,$$

(19) 
$$\frac{\partial}{\partial t} \left\{ m(S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \varepsilon_g) + (1 - m) \rho_s \varepsilon_s \right\} \\ + div \left\{ \rho_w \varepsilon_w \mathbf{V}_w + \rho_g \varepsilon_g \mathbf{V}_g + [P(\mathbf{V}_w + \mathbf{V}_g)] \right\} + div \mathbf{W} + q_\varepsilon = 0,$$

(20) 
$$\mathbf{W} = -\left\{m\left(S_w\lambda_w + (1-S_w)\lambda_g\right) + (1-m)\lambda_s\right\}\nabla T.$$

We exclude the function  $S_w$  from the time derivative of equations (17),(18),(19) and obtain the equations that determine the nonisothermal process of piezoconductivity in the thawed zone:

(21) 
$$\frac{S_w}{\rho_w}\frac{\partial(m\rho_w)}{\partial t} + \frac{1-S_w}{\rho_g}\frac{\partial(m\rho_g)}{\partial t} + DIG = 0,$$

(22) 
$$m\{S_w\rho_w\frac{\partial\varepsilon_w}{\partial t} + (1-S_w)\rho_g\frac{\partial\varepsilon_g}{\partial t}\} + \frac{\partial[(1-m)\rho_s\varepsilon_s]}{\partial t} + DIG_{\varepsilon} = 0.$$

Here, the combination of mass (DIG) and energy  $(DIG_{\varepsilon})$  divergences with the effect of the corresponding sources  $(q_w, q_q, q_{\varepsilon})$  is determined similarly to (14).

2.3. Investigation of saturation transfer block properties. The system (1)-(7) given in subsection 2.1 is a complex quasilinear system of equations of mathematical physics of mixed type. The linearized block of the saturation transfer equations (1)-(4) in it with fixed thermodynamic parameters (P, T) and the absence of capillary and gravitational terms in Darcy laws (3), (4) has hyperbolic properties. This means that grid approximations must be constructed taking into account that they correspond to the hyperbolicity of the system (if it exists) or are simply admissible in its absence. On the other hand, even in the purely hyperbolic case, the application of classical difference schemes that carry the invariants of the hyperbolic system of equations along the characteristics is too cumbersome in the case of modeling gas-hydrate phenomena. After a theoretical analysis of the hyperbolicity of the block of saturation transfer equations (1)-(4) for the direct construction of the regularization of a difference algorithm it seems reasonable to go into an approximate diagonal-characteristic form of writing hyperbolic equations. In this form, both invariants are understood in a simplified way. They, in fact, are the saturations themselves: that  $S_{\nu}$  and water saturation  $S_w$ . Their transfer along the characteristics in the simplest cases is associated respectively with the drift from the direction opposite to the physical movement of the substance (downwind) for  $S_{\nu}$  and from the direction of the movement of the substance (upwind) for  $S_w$ .

Consider the linearization of equations (1)-(4) in the one-dimensional approximation. Direct the X axis along the reservoir.

$$\begin{split} (S_{\nu})_{t}^{'} + \frac{k_{S_{\nu}}^{'}}{\Psi} [\frac{k_{rw}}{\mu_{w}} P_{x}^{'} + \frac{k_{rg}}{\mu_{g}} P_{x}^{'}] (S_{\nu})_{x}^{'} + \frac{k}{\Psi} [\frac{(k_{rw})_{S_{w}}^{'}}{\mu_{w}} P_{x}^{'} + \frac{(k_{rg})_{S_{w}}^{'}}{\mu_{g}} P_{x}^{'}] (S_{w})_{x}^{'} = < \dots >, \\ (S_{w})_{t}^{'} - \frac{k_{S_{\nu}}^{'}}{mS_{\nu}\Psi} [\frac{k_{rw}}{\mu_{w}} P_{x}^{'}\Psi_{g} - \frac{k_{rg}}{\mu_{g}} P_{x}^{'}\Psi_{w}] (S_{\nu})_{x}^{'} - \frac{k}{mS_{\nu}\Psi} [\frac{(k_{rw})_{S_{w}}^{'}}{\mu_{w}} P_{x}^{'}\Psi_{g} - \frac{(k_{rg})_{S_{w}}^{'}}{\mu_{g}} P_{x}^{'}\Psi_{w}] (S_{w})_{x}^{'} = < \dots >, \end{split}$$

Here the stroke denotes the corresponding derivative. In the expressions < ... > there are no spatial-temporal derivatives of saturations  $S_{\nu}$ ,  $S_w$ . For the quantity

$$\frac{\Psi}{m\rho_{\nu}} = \left[\frac{\beta_w}{\rho_w} + \frac{1-\beta_w}{\rho_g}\right] - \frac{1}{\rho_{\nu}} > 0$$

of a jump in the specific volume during the phase decomposition of the unit of mass of the hydrate (see subsection 2.1) it is introduced fragmentation  $\Psi = \Psi_w + \Psi_g$ , exactly,

$$\frac{\Psi_w}{m\rho_\nu} = \frac{\beta_w}{\rho_w} - \frac{S_w}{\rho_v}, \ \frac{\Psi_g}{m\rho_\nu} = \frac{1-\beta_w}{\rho_g} - \frac{1-S_w}{\rho_\nu}.$$

Since a similar linearization in the thawed zone (17), (18) leads to expressions of the form:

$$\begin{split} (S_w)'_t &- \frac{k}{m} [\frac{(k_{rw})'_{S_w}}{\mu_w} P'_x] (S_w)'_x = < \dots >, \\ (S_w)'_t &- \frac{k}{m} [\frac{-(k_{rg})'_{S_w}}{\mu_g} P'_x] (S_w)'_x = < \dots >, \end{split}$$

then the corresponding upwind approximation for water saturation  $S_w$ , the condition of characteristic cross-linking (i.e., one-directionality of characteristics at the transition across the phase boundary) of the hydrate-saturated three-phase and non-hydrated flow regions will be

$$\frac{(k_{rw})'_{S_w}}{\mu_w}\Psi_g - \frac{(k_{rg})'_{S_w}}{\mu_g}\Psi_w > 0.$$

Or more stringent conditions

 $\frac{\Psi_g}{m\rho_{\nu}} > 0, \text{ at } S_w > (S_w)_{min},$   $\frac{\Psi_w}{m\rho_{\nu}} > 0, \text{ at } S_w < (S_w)_{max}.$ 

Here  $k_{rw}(S_w) = 0$  at  $S_w < (S_w)_{min}$  and  $k_{rg}(S_w) = 0$  at  $S_w > (S_w)_{max}$ .

From the point of view of jumps in the specific (per unit mass) phase volume during a phase transition, these requirements can be interpreted as follows. With the complete decomposition of the hydrate mass unit, the volume of the released gas must be greater than  $(1 - S_w)$ , that is the fraction of the volume of the gas hydrate phase. In this case, the volume of released water must be greater than  $S_w$ , that is the fraction of the volume of the gas hydrate phase.

We now introduce the notations

$$\bar{k}_{w} = \frac{k_{rw}}{\mu_{w}} P'_{x}, \ \bar{k}_{g} = \frac{k_{rg}}{\mu_{g}} P'_{x},$$
$$\bar{k}'_{w} = \frac{(k_{rw})'_{S_{w}}}{\mu_{w}} P'_{x}, \ \bar{k}'_{g} = \frac{(k_{rg})'_{S_{w}}}{\mu_{g}} P'_{x}$$

and rewrite the result of three-phase linearization in a more compact form

$$(S_{\nu})_{t}^{'} + \frac{k_{s\nu}}{\Psi} [\bar{k}_{w} + \bar{k}_{g}] (S_{\nu})_{x}^{'} + \frac{k}{\Psi} [\bar{k}_{w}^{'} + \bar{k}_{g}^{'}] (S_{w})_{x}^{'} = < \dots >,$$
  
$$(S_{w})_{t}^{'} - \frac{k_{S_{\nu}}^{'}}{mS_{\nu}\Psi} [\bar{k}_{w}\Psi_{g} - \bar{k}_{g}\Psi_{w}] (S_{\nu})_{x}^{'} - \frac{k}{mS_{\nu}\Psi} [\bar{k}_{w}^{'}\Psi_{g} - \bar{k}_{g}^{'}\Psi_{w}] (S_{w})_{x}^{'} = < \dots >.$$

The eigenvalues  $\lambda$  of the matrix of this system of differential equations composed of the coefficients of the spatial derivatives satisfy the following differential equation.

$$\lambda^{2} - \left[\frac{k_{S_{\nu}}}{\Psi}(\bar{k}_{w} + \bar{k}_{g}) - \frac{k}{mS_{\nu}\Psi}(\bar{k}_{w}\Psi_{g} - \bar{k}_{g}\Psi_{w})\right]\lambda + \frac{kk_{S_{\nu}}^{'}}{mS_{\nu}\Psi}\frac{(p_{x}^{'})^{2}}{\mu_{w}\mu_{g}}[k_{rw}(k_{rg})_{S_{w}}^{'} - k_{rg}(k_{rw})_{S_{w}}^{'}] = 0.$$

Since  $[k_{rw}(k_{rg})'_{S_w} - k_{rg}(k_{rw})'_{S_w}] \leq 0$  (because  $(k_{rg})'_{S_w} \leq 0$ ), the roots  $\lambda$  of the characteristic equation are real and distinct. Moreover, they are different in sign, that is, the block of saturation transfer equations (1) - (4) is hyperbolic and the characteristics are directed in different directions. We also see that on the diagonal of the linearized matrix in the equation for the thawing  $S_{\nu}$  there is a positive value  $\frac{k'_{S_{\nu}}}{\Psi}\left[\frac{k_{rw}}{\mu_{w}} + \frac{k_{rg}}{\mu_{g}}\right] > 0, \text{ which, in accordance with the Darcy laws (3), (4), corresponds to the last of the la$ to a downwind approximation with respect to the thawing  $S_{\nu}$ . Similarly, the diagonal of the linearized matrix in the equation for water saturation  $S_w$  there is a negative value  $-\frac{k}{mS_{\nu}\Psi}\left[\frac{(k_{rw})'_{S_w}}{\mu_w}\Psi_g - \frac{(k_{rg})'_{S_w}}{\mu_g}\Psi_w\right] < 0$ , which, in accordance with Darcy laws (3), (4), corresponds to the upwind approximation in water saturation  $S_w$ . In more complex cases (taking into account gravity, the solid phase of ice in the pores, various types of hydrates, etc.), a linearized analysis of the block of saturation transfer equations can also be carried out similarly to the one above. As a result, monotonization factors  $W_{\phi}(\lambda) > 0$  locally corresponding to various types of saturation approximations (upwind, downwind, symmetric, etc.) in the coefficients of absolute and relative permeabilities are selected on the basis of the spatial grid  $\phi$ , on the edges  $\lambda$  forming them (see Section 3). These factors that tend to unity when grinding the spatial grid  $W_{\phi}(\lambda)$  are corrections on the edges  $\lambda$  to the approximation of the absolute and relative permeabilities in the central nodes of the grid bases (see Section 3). Further, in the work by the method of support operators, vector analysis operations are constructed, which are necessary for approximation of equations (1)-(7) with allowance for some selected monotonizations on the grid for saturation transfer processes (1)-(4).

## 3. The grids of the support operator method

**3.1. Some general information.** The support operators method (SOM) is used for the approximation agreed in the sense of some integral identities, the conjugate operations of vector analysis (div, grad, rot, etc.) necessary for the numerical simulation of mathematical physics problems. In paper [13], divergent difference schemes

were constructed for gas dynamics problems in Lagrangian variables that have the property of component-wise integral conservation of internal and kinetic energies. Mathematically, this became possible due to the approximation on the grid of some integral identity, connecting the operations of vector analysis div and grad. Such schemes began to be called completely conservative. In the future, the cycle of works [3, 6, 7, 14, 15, 16, 17] was associated with the independent development of this idea - the coordinated approximation of pairs of difference operations of vector analysis (div, grad, rot, etc.) due to some integral identities connecting them. The method of obtaining integrally consistent difference schemes with the pairs of conjugate operations of vector analysis included in them became known as the support operator method (SOM). Works in this direction continue to develop, but among those already published we will note two monographs. In [16], SOM is used to solve elliptic-type equations, the heat equation, and Lagrangian gas dynamics problems. Spatially one- and two-dimensional problems on non-orthogonal quadrangular grids are considered. The properties of the resulting difference schemes are investigated on classical solutions. In the monograph [7], in the spatially two-dimensional case on irregular (three- and quadrilateral) grids, the conditions for convergence of difference schemes of the SOM with first order for the Poisson equation and the equations of the linear theory of elasticity on classical and generalized solutions are established. These conditions can be interpreted as some requirements of the closure of surfaces around the nodal domains of the grid metrically conjugated to the original grid cells (see Fig. 5). In [6], for constructed SOM algorithms of arbitrary dimension (including for tetrahedral grids) as applied to divergent-gradient problems and linear elasticity theory, the requirements for the closedness of a metrically conjugate grid, which are similar to the spatial two-dimensional solution and are the convergence condition for the difference solution, are generalized. Also in [7], variational difference schemes of Lagrangian gas dynamics are studied on irregular grids. It should be noted that the construction of the same vector analysis operations (div, grad, rot, etc.) using SOM, but in different problems of mathematical physics has its own specifics and may be different. So the base operator SOM in problems with the presence of physical fields (gravitational, electromagnetic) when calculating the forces acting on the particles of the medium (Lorentz) is chosen involuntarily from the approximation of the Gauss or Stokes theorems on the grid cells, and following the variation of the gravitational or electromagnetic energy of the physical process [17]. The application of SOM to filtration problems in sedimentary basins and poroelasticity (the Bio problem) is presented in [3, 4]. Let us stop on this in somewhat more detail. In the upper part of Fig. 3, the geological profile of the Varandey-Adzvinskaya structural zone is presented, while in the lower part of this figure its grid approximation is performed by a body of simple geometry.

This zone has a length of 70 km with a depth of 5 km and a transverse size of 20 km. Different colors are represented by discontinuous and geometrically complex structured reservoir properties of layers, including geological shear deformations. To study the processes of secondary migration of hydrocarbons in relation to the study of the mechanisms of formation of hydrocarbon deposits in this region, numerical modeling (SOM) of the two-phase filtration process of hydrothermal waters and gas has been carried out.

Figure 4 shows the sequential advancement of the hydrocarbon fluid and filling the traps. Initially, the medium was filled only with water. In the lower part of the region, the boundary was set to a fluid flow containing the gas phase with some



FIGURE 1. Geological profile of the Varandey-Adzvinskaya structure zone (above):  $K_1$ -Q - Lower Cretaceous-Quaternary, J -Jurassic,  $T_3$  - Upper Triassic,  $P_2$  - Upper Permian,  $P_1$  - Lower Permian,  $C_1$ - $P_1$  - Lower Carboniferous-Lower Permian,  $D_3$  - Upper Devonian,  $D_2$  - Mid Devonian,  $S_1$  - Lower Devonian Ordovician, D - Devonian, S - Silurian, T-P - Triassic-Permian; grid approximation of the upper profile (bottom).

amplitude. Over a period of 100 years, the gas-fluid impulse reaches the surface layers. The figure 2 shows the distribution of water saturation and it can be seen that if the fluid impulse encounters fluid-impedances on its route, a hydrocarbon deposit is formed. If there is no fluid-impedances, then the impulse is dissipated in the atmosphere. Using the example of the above-described modeling, we see that applying SOM to filtration and elasticity tasks in sedimentary basins requires the ability to work with discontinuous physical properties of the substance, irregular grids that simulate, in particular, shear zones and multiscale adaptation.

On these coarse grids, it is required not to lose the qualitative approximation of saturation transfer processes in the medium and the thermodynamic gradients of the discontinuities in the material properties of the medium. Also, the difference model can approximate the identities of SOM at different layers in time and in this case special interpolation technologies of these identities in time may be required. For example, in section 4 in this situation, free volume weighing is applied. Below, the work describes the SOM algorithms, taking into account the above specifics of



FIGURE 2. Sequential advancement of hydrocarbon fluid and filling traps. The color indicates the water saturation distribution  $S_w$ .

the filtration problems and the technical features that are present in the modeling of piezoconductive processes with solid-phase inclusions.

**3.2.** SOM for piezoconductive problems with solid phase inclusions. The results of this section are similar to those presented in [8], where the processes in the thawed zone were not considered.

The presence of a closed conjugate ("shifted") grids consisting, for example, of domains  $d(\omega)$  around nodes  $\omega$  (see Fig.3) is typical for the grids of SOM consisting of cells ( $\Omega$ ) formed by nodes ( $\omega$ ), faces ( $\sigma$ ), and edges ( $\lambda$ ).

The metric grid operator  $\boldsymbol{\sigma}(\lambda) = \sum_{\varphi(\lambda)} V_{\varphi} \mathbf{e}'_{\varphi}(\lambda)$  (see also below) determines the faces of the node domain. Here, the bases  $\varphi(\lambda)$  are in pairs in the cells  $\Omega(\lambda)$  adjacent

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to the edge  $\lambda$ . The metric calibration of the difference grid consists in choosing the volumes of bases (with the natural normalization condition  $\sum_{\varphi(\Omega)} V_{\varphi} = V_{\Omega}$ ). It defines the construction of a closed conjugate mesh for various classes of grids.

These are the triangular-quadrangular 2D grids, tetrahedral, parallelepiped, prismatic, etc. 3D grids and their mortar stitches, their adaptation (with the introducing the new nodes in the cells  $\Omega$ ) with preservation of self-adjointness and signdefiniteness of the corresponding "divergent-gradient" operations of vector analysis of continuous boundary value problems. The further presentation is general. The example of a triangular-quadrangular 2D grid illustrates the specific choice of local basis volumes  $V_{\varphi}$ .

We introduce a family of irregular difference grids in the region O. We consider the case when the grid consists of triangular and quadrangular cells  $(\Omega)$ , bases  $(\varphi)$ , nodes  $(\omega)$ , edges  $(\lambda)$ , and related to them the boundaries  $(\sigma (\lambda))$  of the node balance domains  $d(\omega)$  (see Fig.3).



FIGURE 3. Construction of bases.

The system of initial (covariant) unit vectors  $\mathbf{e}(\lambda)$  created by the edges forms the bases  $\varphi$ . We accept the centers of cells  $\Omega$  and edges  $\lambda$  like the arithmetic mean of radius vectors of their nodes  $\omega$ . The curve is a surface that connects these centers (two adjacent cells through an edge or a cell with a boundary edge  $\partial \lambda$ )

$$\boldsymbol{\sigma}(\lambda) = \sum_{\varphi(\lambda)} \mathbf{v}_{\varphi} \mathbf{e}'_{\varphi}(\lambda)$$

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

The internal divergence of a vector field  $DIN_w : (\varphi) \to (\omega)$  is defined by approximating of the Gauss's theorem on  $d(\omega)$ :

$$DIN_{w} \mathbf{X} = \sum_{\lambda(\omega)} s_{\lambda}(\omega) \tau_{wX}(\lambda),$$
  
$$\tau_{wX}(\lambda) = \sum_{\varphi(\lambda)} v_{\varphi}(\mathbf{e}'_{w\varphi}(\lambda), \mathbf{X}_{\varphi}),$$
  
$$\mathbf{e}'_{w\varphi}(\lambda) = W_{\varphi}(\lambda) \cdot \mathbf{e}'_{\varphi}(\lambda).$$

Here  $\sum_{\lambda(\omega)}$  is the summation over all edges  $\lambda$  having a common node  $\omega$ .

The grid vector field  $\mathbf{X}$  is given by its representations in the bases  $\mathbf{X}_{\varphi}$ . The multipliers  $W_{\varphi}(\lambda) > 0$  given in the bases  $\varphi$  on the edges  $\lambda(\varphi)$  formed them relate to the monotonization of the grid solutions in the following sense. The approximation of absolute permeability  $k(S_{\nu})$  is selected downwind in accordance with the analysis of the hyperbolicity of the linearized group of equations (1), (2) for saturations in the absence of gravity and at fixed pressure and temperature. Relative permeabilities  $k_{rw}(S_w)$  and  $k_{rg}(1-S_w)$  are taken upwind. It is taken into account when choosing factors  $W_{\varphi}(\lambda)$ . The absence of an index, written as w in expressions  $DIN_w\mathbf{X}$ ,  $\tau_{wx}(\lambda)$ ,  $\mathbf{e'}_{w\varphi}$  and  $GRAD_wu$ , automatically denotes  $W_{\varphi}(\lambda) = 1$  in all bases  $\varphi$  on the edges  $\lambda(\varphi)$  formed them. It means the absence of monotonization of the grid solution in the approximations used in the above sense.

We use ( )<sub> $\Delta$ </sub> to denote the approximation of the corresponding differential expressions and have:

$$(\int_{O} (\mathbf{X}, \nabla u) \, dv)_{\Delta} = -(\int_{O} u \, \operatorname{div} \mathbf{X} dv - \int_{\partial O} u \, (\mathbf{X}, \, d\mathbf{s}))_{\Delta}$$
$$= -\sum_{\omega} (u_{\omega}, \operatorname{DIN}_{w} \mathbf{X}) = \sum_{\varphi} v_{\varphi} (\mathbf{X}_{\varphi}, \, \operatorname{GRAD}_{w} u).$$

Gradient vector field  $GRAD_w : (\omega) \to (\varphi)$  is given by its representations in bases:

$$GRAD_w u = \sum_{\lambda(\varphi)} \Delta_\lambda u \mathbf{e'}_{w\varphi}(\lambda), \ \Delta_\lambda u = -\sum_{\omega(\lambda)} s_\lambda(\omega) u_\omega = u_{\omega^*} - u_\omega.$$

We assume a vector field  $\mathbf{X}_{w\varphi} = K_{\varphi} \text{GRAD}_{w} u$  as  $\mathbf{X}_{\varphi}$  in the bases  $\varphi$  and we obtain a self-adjoint nonnegative operator  $-DIN_{w}\mathbf{X}_{w}: (\omega) \to (\omega)$  or  $-DIN_{w}K \, GRAD_{w}:$  $(\omega) \to (\omega)$ . Here the flow vector field  $\mathbf{X}_{w}$  is given by its components in the bases  $\mathbf{X}_{w\varphi}$ . This flow vector field is determined by the gradient properties of the scalar grid function u and the grid symmetric positive definite tensor field of conductivity K. This scalar grid function u is given at the nodes  $\omega$  and this tensor K is given by their representations in the bases  $K_{\varphi}$ . This operator will be strictly positive if the first boundary value problem is specified at least in one boundary node of a connected difference grid, i.e. the scalar grid function becomes zero in this boundary node.

It is also considered that the multipliers of the grid solution monotonization tend to be unity with an increase in the approximation, i.e.  $W_{\varphi}(\lambda) \to 1$ . Moreover, the operator  $-DIN_{w}K \ GRAD : (\omega) \to (\omega)$  becomes close to a self-adjoint nonnegative operator  $DIN \ K \ GRAD : (\omega) \to (\omega)$ , although it is not self-adjoint and nonnegative in the strict sense (with the exception of an orthogonal grid).

Cells consisting of orthogonal bases do not violate the properties of self-adjointness and sign-definiteness of the operator  $\text{DIN}_w$ , GRAD in the strict sense, despite the presence in their bases the approximate monotonization of the grid solution.

We consider two families of approximations to preserve the properties of selfadjointness and the sign-definiteness of this operator.

**3.3. Schemes with limited monotonization of the grid solution.** We select the set of grid cells  $(\Omega^*)$  in which there is at least one non-orthogonal basis  $\varphi$ formed by the edges  $(\lambda(\varphi))$ .  $W_{\varphi}(\lambda) = 1$  is considered in all bases  $(\varphi(\Omega^*))$  within these cells  $\Omega^*$  (i.e. can be orthogonal). I.e. the monotonization of the grid solution is absent in these bases. For example, the dependence of the representation of the tensor field of conductivity  $K_{\varphi}$  on "hyperbolic" variables (hydrate thaw  $S_{\nu}$ , water saturation  $S_w$ , etc.) is approximated directly at the central node  $\omega$  of the grid forming the basis  $\varphi$ . Such schemes have a self-adjoint and a sign-definite operator  $DIN_w K \ GRAD : (\omega) \to (\omega)$ . However, they do not have the monotonization on the set of grid cells containing non-orthogonality.

**3.4.** Quasimonotone schemes. We denote the set of non-orthogonal grid bases as  $(\varphi^*)$ . Correspondingly,  $(\varphi)/(\varphi^*)$  are orthogonal bases. We introduce  $\mathbf{X}_{w\varphi}$ 

 $GRAD_{w}^{*}u = \begin{cases} GRADu, \ \varphi \in (\varphi)/(\varphi*) \\ GRAD_{w}u, \ \varphi \in (\varphi*) \end{cases} \text{ to approximate a vector field } \mathbf{X} = K \text{ grad } u.$ 

These schemes have self-adjoint and sign-definite operator  $DIN_wK\;GRAD^*_w$  :  $(\omega) \to (\omega)$ . Since, the multipliers of the grid solution monotonization tend to be unity with increasing approximation, i.e.  $W_{\varphi}(\lambda) \to 1$ , then the operators  $GRAD_w$ :  $(\omega) \to (\varphi)$  and  $GRAD : (\omega) \to (\varphi)$  approximate the differential operator grad. The quasimonotone schemes with self-adjointness and the sign-definiteness of the operator  $DIN_w K \, GRAD_w^* : (\omega) \to (\omega)$  in nonorthogonal grid bases  $(\varphi^*)$  save monotonicity in contradistinction to schemes with limited monotonization when calculate fluxes in conjugate basis directions.

Approaches 1 and 2 can be applied locally, i.e. only in the part of non-orthogonal bases  $(\varphi * *)$ , where the condition  $(GRADu, GRAD_w u) \geq 0$  is not met at the "predictor" stage (explicit time layer, known iteration, etc.). An appropriate set of cells  $(\Omega^{**})$  is generated for schemes with limited monotonization in the formation of which at least one basis of  $(\varphi * *)$  took part. 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, the preservation of the sign-definiteness of quadratic forms is useful for physical applications because it allows to correctly approximate the exact square of the gradient of the thermodynamic quantities in the depression wells, in particular, the Joule-Thomson effect in the nonisothermal filtration processes considered below.

In the model of the filtration fluid dynamics with gas hydrate inclusions, the mechanism of monotonization of the grid solution  $W_{\varphi}(\lambda) > 0$ , taking into account the hyperbolicity (with no gravity, g = 0) of the system (1), (2) investigated in , provides effective monotonization of the grid solution on  $S_{\nu}, S_w$  and  $S_q = 1 - S_w$ . Also, this mechanism ensures the preservation of the sign-definiteness of the quadratic forms of the gradients of thermodynamic quantities in the piezoconductive part of the discrete connected task of nonisothermal filtration considered below.

According to the studies of , the absolute permeability  $k(S_{\nu})$  in the bases  $\varphi$  on the edges  $(\lambda(\varphi))$  forming these bases is always chosen downwind (along thaw). Relative permeabilities  $k_{rw}(S_w)$  and  $k_{rg}(1-S_w)$ , as a rule, are taken upwind (along water and gas saturation), i.e. as in a two-phase thawed zone with no hydrate. However, in accordance with the stability conditions analyzed in, a change in the sign of the directwind (i.e, downwind along the water and gas saturations) is also possible here.

## 4. Free-volume approximation of divergent-piezoconductive difference schemes in the thawed zone and the medium with gas hydrate inclusions

4.1. Three-phase medium with hydrate inclusions. We introduce some notation for the grid functions of the support operator method (Section 3, see also Fig.3). We will refer to its nodes  $\omega$  previously presented in the continuum model quantities

 $\overline{m}, S_{\nu}, S_{w}, \rho_{\nu}, \rho_{w}, \rho_{g}, \rho_{s}, P, T, \varepsilon_{\nu}, \varepsilon_{w}, \varepsilon_{g}, \varepsilon_{s}, \mu_{w}, \mu_{g}, k_{rw}, k_{rg}, q_{w}, q_{g}, q_{\varepsilon}.$ 

We assign the vector functions to the grid bases  $\varphi$  in accordance with Section 3

$$\mathbf{V}_w, \mathbf{V}_a, \nabla P, \nabla T, \mathbf{W}.$$

We assign the grid functions that represent the discontinuous material properties of substances to cells  $\Omega$ 

$$m, k, \lambda_{\nu}, \lambda_{w}, \lambda_{g}, \lambda_{s}.$$

The relations are obvious

$$\overline{m_{\omega}} = \sum_{\varphi(\omega)} V_{\varphi} m_{\Omega(\varphi)}, \quad \overline{(1-m)_{\omega}} = \sum_{\varphi(\omega)} V_{\varphi} (1-m_{\Omega(\varphi)}) = V_{\omega} - \overline{m_{\omega}}, \quad V_{\omega} = \sum_{\varphi(\omega)} V_{\varphi},$$

i.e.  $\overline{m_{\omega}}$  and  $\overline{(1-m)_{\omega}}$  represent the volume of the pore domain  $d(\omega)$  (see Fig.3) and its frame part, respectively.

Then, we introduce the difference derivatives on time and the space-point (in grid nodes  $\omega$ ) time interpolations  $a_t = (\hat{a} - a)/\tau$ ,  $a^{(\delta)} = \delta \hat{a} + (1 - \delta)a$  on the time layers t and  $\hat{t} = t + \tau$  ( $\tau > 0$  is the time step). Here the interpolation weight  $\delta$  may depend on the spatial grid node  $\omega$ .

Under the value

$$\delta_{\nu} = \sqrt{(\overline{m}S_{\nu})^{\uparrow}} / \left( \sqrt{(\overline{m}S_{\nu})^{\uparrow}} + \sqrt{(\overline{m}S_{\nu})} \right), \ 0 < S_{\nu} < 1,$$

we mean the free-volume time approximation of the grid functions given at the nodes  $\omega$ , i.e. interpolation weight  $\delta_{\nu}$  is determined by the proportion of the pore volume, intended for free movement of the liquid and gas. The choice of such an approximation allows us to produce discrete transformations of equations related to their splitting by physical processes, close to continual ones. Other arbitrary interpolations with respect on time will be denoted by []  $\sim$ . They can relate not only to grid nodes  $\omega$ , but also to its other elements (bases  $\varphi$  and etc.).

We understand by index S in vector analysis operations  $DIN_s$  and  $GRAD_s$  one of the types of monotonization of the grid solution described above (or its absence) monotonizing the transfer by saturation  $S_w$  and  $S_\nu$  and 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

(23) 
$$\left\{\overline{m}\left[S_{\nu}S_{w}\rho_{w}+(1-S_{\nu})\rho_{\nu}\beta_{w}\right]\right\}_{t}+DIN_{s}(\rho_{w}\mathbf{V}_{w})^{\sim}+q_{w}^{\sim}=0,$$

(24) 
$$\{\overline{m} [S_{\nu}(1-S_w)\rho_g + (1-S_{\nu})\rho_v(1-\beta_w)]\}_t + DIN_s(\rho_g \mathbf{V}_g)^{\sim} + q_g^{\sim} = 0.$$

With the help of the operator  $GRAD_s$ , fluxes of water  $(\rho_w \mathbf{V}_w)^{\sim}$  and gas  $(\rho_g \mathbf{V}_g)^{\sim}$  are approximated in grid bases  $\varphi$  taking into account the discretization of Darcy's law (3), (4), for example, on the implicit time layer by any of the standard methods [4, 6].

$$\begin{split} (\rho_w \mathbf{V}_w)_{\varphi}^{p\sim} &= -\left(\rho_w \frac{kk_{rw}}{\mu_w}\right)_{\underline{\Delta}\varphi}^{\sim} GRAD_s P^{\sim} + \left(\rho_w^2 \frac{kk_{rw}}{\mu_w}\right)_{\underline{\Delta}\varphi}^{\sim} g\mathbf{k}, \\ (\rho_g \mathbf{V}_g)_{\varphi}^{p\sim} &= -\left(\rho_g \frac{kk_{rg}}{\mu_g}\right)_{\underline{\Delta}\varphi}^{\sim} GRAD_s P^{\sim} + \left(\rho_g^2 \frac{kk_{rg}}{\mu_g}\right)_{\underline{\Delta}\varphi}^{\sim} g\mathbf{k}. \end{split}$$

Here we mean under ()  $\underline{\Delta}_{\varphi}$  the approximations of the corresponding expressions in grid bases  $\varphi$  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  $\int \varepsilon div(\rho \mathbf{V}) dV$  (see also (27) 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 the following can be written

$$d\varepsilon_w = \varepsilon_{wp}^{'} dP, \ d\varepsilon_g = \varepsilon_{gp}^{'} dP,$$

where  $\varepsilon'_{wp}$  and  $\varepsilon'_{gp}$  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  $\varphi$  (formed by the nodes in which the thermobaric relation (7) is satisfied) can be represented in the energy form:

$$\begin{split} (\rho_w \mathbf{V}_w)_{\varphi}^{\varepsilon \sim} &= -\left(\rho_w \frac{kk_{rw}}{\mu_w \varepsilon'_{wp}}\right)_{\underline{\Delta}\varphi}^{\sim} GRAD_s \varepsilon_w^{(\delta_v)} + \left(\rho_w^2 \frac{kk_{rw}}{\mu_w}\right)_{\underline{\Delta}\varphi}^{\sim} g\mathbf{k}, \\ (\rho_g \mathbf{V}_g)_{\varphi}^{\varepsilon \sim} &= -\left(\rho_g \frac{kk_{rg}}{\mu_g \varepsilon'_{gp}}\right)_{\underline{\Delta}\varphi}^{\sim} GRAD_s \varepsilon_g^{(\delta_v)} + \left(\rho_g^2 \frac{kk_{rg}}{\mu_g}\right)_{\underline{\Delta}\varphi}^{\sim} g\mathbf{k}. \end{split}$$

In this way

$$(\rho_w \mathbf{V}_w)_{\varphi}^{\sim} = \{(\rho_w \mathbf{V}_w)_{\varphi}^{p\sim} | (\rho_w \mathbf{V}_w)_{\varphi}^{\varepsilon\sim}\}, \ (\rho_g \mathbf{V}_g)_{\varphi}^{\sim} = \{(\rho_g \mathbf{V}_g)_{\varphi}^{p\sim} | (\rho_g \mathbf{V}_g)_{\varphi}^{\varepsilon\sim}\}.$$

The equation for the balance of internal energy approximating (5) has the form:

$$\left\{ \overline{m} \left[ S_{\nu} \left( S_{w} \rho_{w} \varepsilon_{w} + (1 - S_{w}) \rho_{g} \varepsilon_{g} \right) + (1 - S_{\nu}) \rho_{\nu} \varepsilon_{\nu} \right] + \overline{(1 - m)} \rho_{s} \varepsilon_{s} \right\}_{t} + \\ + DIN_{s} \left[ \left( \varepsilon_{w}^{(\delta_{\nu})} \right)_{up} \left( \rho_{w} \mathbf{V}_{w} \right)^{\sim} \right] + DIN_{s} \left[ \left( \varepsilon_{g}^{(\delta_{\nu})} \right)_{up} \left( \rho_{g} \mathbf{V}_{g} \right)^{\sim} \right] + \\ + DIN \left\{ \left[ P \left( \mathbf{V}_{w} + \mathbf{V}_{g} \right) \right]^{\sim} \right\} + DIN \mathbf{W}^{\sim} + q_{\varepsilon}^{\sim} = 0.$$

Index up in the expression for the energy of water  $(\varepsilon_w^{(\delta_\nu)})_{up}$  indicates that the respective values are taken up (upwind) by the water flux  $(\rho_w \mathbf{V}_w)^\sim$  in a previously defined divergence  $DIN_s(\rho_w \mathbf{V}_w)^\sim$ . Similarly, the index up is understood in the expression for the energy of the gas  $(\varepsilon_a^{(\delta_\nu)})_{up}$ .

expression for the energy of the gas  $(\varepsilon_g^{(\delta_{\nu})})_{up}$ . Work of pressure forces  $[P(\mathbf{V}_w + \mathbf{V}_g)]^{\sim}$  and the total heat flux  $\mathbf{W}^{\sim}$  in the medium are approximated in grid bases  $\varphi$ , for example, on the implicit time layer in a standard way [4, 6]:

$$[P(\mathbf{V}_w + \mathbf{V}_g)]_{\varphi}^{\sim} = \left(\frac{P}{\rho_w}\right)_{\varphi}^{\sim} (\rho_w \mathbf{V}_w)_{\varphi}^{p\sim} + \left(\frac{P}{\rho_g}\right)_{\varphi}^{\sim} (\rho_g \mathbf{V}_g)_{\varphi}^{p\sim}.$$

Further, the discrete analogue of the piezoconductive equation (14) physically split with the saturation block (23), (24), but difference-equivalent to the system

of conservation laws of the model (23), (24), (25) has the form:

$$\delta_{\varepsilon}^{(\delta_{\nu})} \{ [(\overline{m}S_{\nu})S_{w}]^{(1-\delta_{\nu})} \frac{(\rho_{w})_{t}}{(\rho_{w})^{(\delta_{\nu})}} + [(\overline{m}S_{\nu})(1-S_{w})]^{(1-\delta_{\nu})} \frac{(\rho_{g})_{t}}{(\rho_{g})^{(\delta_{\nu})}} + [\overline{m}(1-S_{\nu})]^{(1-\delta_{\nu})} \frac{(\rho_{\nu})_{t}}{(\rho_{\nu})^{(\delta_{\nu})}} + (\overline{m})_{t} \} + [\psi/(m\rho_{\nu})]^{\sim} \{ [(\overline{m}S_{\nu})S_{w}\rho_{w}]^{(1-\delta_{\nu})} (\varepsilon_{w})_{t} + [(\overline{m}S_{\nu})(1-S_{w})\rho_{g}]^{(1-\delta_{\nu})} (\varepsilon_{g})_{t} + [\overline{m}(1-S_{\nu})\rho_{\nu}]^{(1-\delta_{\nu})} (\varepsilon_{\nu})_{t} + [\overline{(1-m)}\rho_{s}\varepsilon_{s}]_{t} \} + \delta_{\varepsilon}^{(\delta_{\nu})}DIG^{\sim} + [\psi/(m\rho_{\nu})]^{\sim}DIG^{\sim}_{\varepsilon} = 0,$$

$$\delta_{\varepsilon} = \left[\beta_{w}\varepsilon_{w} + (1 - \beta_{w})\varepsilon_{g}\right] - \varepsilon_{\nu},$$

$$\left[\psi/(m\rho_{\nu})\right]^{\sim} = \left[\beta_{w}/(\rho_{w})^{(\delta_{\nu})} + (1 - \beta_{w})/(\rho_{g})^{(\delta_{\nu})}\right] - 1/(\rho_{\nu})^{(\delta_{\nu})},$$

$$DIG^{\sim} = \frac{1}{(\rho_{w})^{(\delta_{\nu})}}DIN_{s}(\rho_{w}\mathbf{V}_{w})^{\sim} + \frac{1}{(\rho_{g})^{(\delta_{\nu})}}DIN_{s}(\rho_{g}\mathbf{V}_{g})^{\sim} + \frac{q_{w}^{\sim}}{(\rho_{w})^{(\delta_{\nu})}} + \frac{q_{g}^{\sim}}{(\rho_{g})^{(\delta_{\nu})}},$$

$$DIG^{\sim}_{\varepsilon} = \left[DIN_{s}\left\{(\varepsilon_{w}^{(\delta_{\nu})})_{up}(\rho_{w}\mathbf{V}_{w})^{\sim}\right\} - (\varepsilon_{w})^{(\delta_{\nu})}DIN_{s}(\rho_{w}\mathbf{V}_{w})^{\sim}\right] + \left[DIN_{s}\left\{(\varepsilon_{g}^{(\delta_{\nu})})_{up}(\rho_{g}\mathbf{V}_{g})^{\sim}\right\} - (\varepsilon_{g})^{(\delta_{\nu})}DIN_{s}(\rho_{g}\mathbf{V}_{g})^{\sim}\right]$$

$$(27) + DIN\left\{\left[P\left(\mathbf{V}_{w} + \mathbf{V}_{g}\right)\right]^{\sim}\right\} + DIN\mathbf{W}^{\sim} + \left(q_{\varepsilon}^{\sim} - \varepsilon_{w}^{(\delta_{\nu})}q_{w}^{\sim} - \varepsilon_{g}^{(\delta_{\nu})}q_{g}^{\sim}\right).$$

In the expression  $DIG_{\varepsilon}^{\sim}$ , which appears in (26), there is a monotonic (upwind) energy approximation for  $\varepsilon_w^{(\delta_\nu)}$  and  $\varepsilon_g^{(\delta_\nu)}$  in the corresponding combinations of divergent expressions containing these quantities.

**4.2. Two phase thawed zone.** Similar to Section 4.1, we obtain a two-phase family of completely conservative difference schemes in the thawed zone, setting the grid function  $S_{\nu} = 1$  at the nodes  $\omega$ . The weight  $\delta_1 = \sqrt{(\overline{m})^2} / \left(\sqrt{(\overline{m})^2} + \sqrt{(\overline{m})}\right)$  is respectively entered at the grid nodes  $\omega$ , instead of interpolation weight  $\delta_{\nu}$ .

The continuity equations, which are the mass balance of the water and gas components in the thawed zone, are written as:

(28) 
$$\{\overline{m}S_w\rho_w\}_t + DIN_s(\rho_w\mathbf{V}_w)^{\sim} + q_w^{\sim} = 0,$$

(29) 
$$\left\{\overline{m}(1-S_w)\rho_g\right\}_t + DIN_s(\rho_g \mathbf{V}_g)^{\sim} + q_q^{\sim} = 0.$$

In the thawed zone, with the help of an operator  $GRAD_s$ , the flow of water  $(\rho_w \mathbf{V}_w)^{\sim}$  and the flow of gas  $(\rho_g \mathbf{V}_g)^{\sim}$  are determined in a non-energy formulation, i.e. they are approximated in the bases  $\varphi$  of the grid by the quantities  $(\rho_w \mathbf{V}_w)_{\varphi}^{p\sim}$  and  $(\rho_g \mathbf{V}_g)_{\varphi}^{p\sim}$ , respectively (see Section 4.1).

The equation of internal energy balance in the thawed zone, approximating (19), has the form:

$$\left\{ \overline{m} \left( S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \varepsilon_g \right) + \overline{(1 - m)} \rho_s \varepsilon_s \right\}_t + \\ + DIN_s \left[ \left( \varepsilon_w^{(\delta_1)} \right)_{up} \left( \rho_w \mathbf{V}_w \right)^{\sim} \right] + DIN_s \left[ \left( \varepsilon_g^{(\delta_1)} \right)_{up} \left( \rho_g \mathbf{V}_g \right)^{\sim} \right] + \\ + DIN \left\{ \left[ P \left( \mathbf{V}_w + \mathbf{V}_g \right) \right]^{\sim} \right\} + DIN \mathbf{W}^{\sim} + q_{\varepsilon}^{\sim} = 0.$$
(30)

The designation and understanding of difference objects (indices up, s, work of pressure forces, heat flux) are the same as in the corresponding analogues in Section 4.1.

Further, we exclude the function  $S_w$  defined in the grid nodes  $\omega$  from the sign of the difference time derivative and we obtain completely conservative difference equations that determine the non-isothermal process of piezoconductivity in the thawed zone from equations (28),(29),(30):

(31) 
$$\frac{\left(S_w\right)^{\left(\delta_1\right)}}{\left(\rho_w\right)^{\left(\delta_1\right)}} \left[\overline{m}\rho_w\right]_t + \frac{\left(1 - S_w\right)^{\left(\delta_1\right)}}{\left(\rho_g\right)^{\left(\delta_1\right)}} \left[\overline{m}\rho_g\right]_t + DIG^{\sim} = 0,$$

(32) 
$$(\overline{m})^{(1-\delta_1)} \{ [S_w \rho_w]^{(\delta_1)} (\varepsilon_w)_t + [(1-S_w) \rho_g]^{(\delta_1)} (\varepsilon_g)_t \} + \left[ \overline{(1-m)} \rho_s \varepsilon_s \right]_t + DIG_{\varepsilon}^{\sim} = 0.$$

The combination of mass difference  $(DIG^{\sim})$  and energy  $(DIG_{\varepsilon})$  divergences in the nodes  $\omega$  together with the action of the corresponding sources  $(q_{w}^{\sim}, q_{g}^{\sim}, q_{\varepsilon}^{\sim})$  are determined similarly to (27), but with changing the interpolation weight  $\delta_{\nu}$  to the weight  $\delta_{1}$ .

## 5. Algorithms for the joint calculation of hydrate-containing and thawed states of a fluid-dynamic medium

We match a fixed unit volume and the whole mass of water molecules  $M_w$ , the mass of methane molecules  $M_g$ , and the total internal energy E of the system, including the skeleton, located in this volume, to the node balanced domain  $d(\omega)$  of the grid. Then, the local thermodynamic equilibrium state of the medium is uniquely determined, according to the parameters  $\{1, M_w, M_g, E\}$ . We also assume that the range of variation of the balance parameters  $\{M_w, M_g, E\}$  is such that either a thawed zone or a three-phase hydrate-containing medium occurs.

Therefore, either a solution  $\{S_{\nu}, S_w, P, T\}$  in a three-phase hydrate-containing thermodynamic equilibrium state, or a solution  $\{S_w, P, T\}$  corresponding to the thermodynamic equilibrium two-phase thawed zone are the mandatory alternative. Further, we consider separately these two tasks.

5.1. Three-phase hydrate-containing state. The balance equations for the mass of water  $M_w$ , the mass of methane  $M_g$  and the total internal energy of the system E in a single node volume (with porosity  $m_{\omega} = \overline{m}_{\omega}/V_{\omega}$ ) are:

(33) 
$$m \left[ S_{\nu} S_{w} \rho_{w} + (1 - S_{\nu}) \rho_{\nu} \beta_{w} \right] = M_{w},$$

(34) 
$$m \left[ S_{\nu} (1 - S_w) \rho_g + (1 - S_{\nu}) \rho_{\nu} (1 - \beta_w) \right] = M_g,$$

(35)  $m \left[ S_{\nu} \left( S_{w} \rho_{w} \varepsilon_{w} + (1 - S_{w}) \rho_{g} \varepsilon_{g} \right) + (1 - S_{\nu}) \rho_{\nu} \varepsilon_{\nu} \right] + (1 - m) \rho_{s} \varepsilon_{s} = E.$ 

In addition, the thermobaric ratio  $T_{dis} = f(P)$  is fulfilled.

The expression  $i_l = c_{pl}T$ , l = g, w, s is fulfilled for the enthalpies of the mass unit  $i_l = \varepsilon_l + P/\rho_l$ ,  $l = g, w, \nu, s$ , where  $c_{pl}$  are the corresponding specific heat capacities at constant pressure.

The enthalpies of hydrate, free water, and gas are thermodynamically consistent in the relation  $\beta_w i_w + (1 - \beta_w)i_g = i_\nu + h$ , where h is the latent heat of the phase transition of the hydrate mass unit. The accounting for the nonideality of the gas can be performed by replacing the heat capacity  $c_{pg}$  with  $i_g/T$  in the lower input thawed heat capacities  $\Phi_p$  and  $f_{pk}$  (see Section 5.3), if the function  $i_g(P,T)$  is known. The same applies to replacing  $c_{pw}$  with  $i_w/T$  and  $c_{ps}$  with  $i_s/T$  in those cases when the enthalpy is disproportionate to the temperature of the medium. For example, the heat capacity of the simple skeleton  $c_{ps}$  is replaced by  $i_k/T$  in the below considered model of a double skeleton of the medium (see Section 5.3), interpreted as a two-phase thawed zone (see (56)).

(36) 
$$\Phi_p = M_w c_{pw} + M_g c_{pg} + (1-m) \rho_s c_{ps} > 0.$$

Here  $\Phi_p$  is the thawed heat capacity at constant pressure of the system per unit volume of medium.

We obtain the equation for the equilibrium pressure P in the system, excluding the functions of thaw  $S_{\nu}$  and water saturation  $S_w$  in the system of equations (33), (34), (35), after simple transformations:

(37) 
$$-\Phi_p + \frac{1}{T} \left[ P + E + \frac{\psi_h}{\psi_\rho} \rho_\nu h \right] = 0,$$

38) 
$$\psi_h = -(m\rho_w - M_w)\rho_q + M_q\rho_w, \ (m\rho_w - M_w) > 0,$$

(39) 
$$\psi_{\rho} = -(\rho_w - \beta_w \rho_{\nu})\rho_q + (1 - \beta_w)\rho_{\nu}\rho_w, \ (\rho_w - \beta_w \rho_{\nu}) > 0.$$

On the solution of the system (33), (34), (35) the relation is satisfied:

(40) 
$$\psi_h = m \left(1 - S_\nu\right) \psi_\rho.$$

It allows to determine the thaw  $S_v$  according to the given thermodynamic parameters of the environment P and  $T = T_{dis} = f(P)$ , and then, for example, from equation (33), to find water saturation  $S_w$ .

The initial approximation  $P_* \in (P_i, P_a)$  and the physically acceptable pressure range  $(P_i < P_a)$ , in which the solution exists and is unique, are assumed to be given for the iterative process (37), (38), (39) of definition of pressure P. We also note the relations which follow from (38), (39):

$$\rho_{g}|_{\psi_{\rho}=0} = \frac{1-\beta_{w}}{\rho_{w}/\rho_{\nu}-\beta_{w}}\rho_{w} < \rho_{w},$$
  
$$\psi_{h}|_{\psi_{\rho}=0} = [M_{g} - \chi_{w} (1-\beta_{w})]\rho_{w}, \ \chi_{w} = (m\rho_{w} - M_{w})/(\rho_{w} - \beta_{w}\rho_{\nu}) > 0.$$

**5.1.1. Ideal gas approximation.** We consider for methane the case of an ideal gas, assuming in (12) a supercompressibility coefficient  $z_g = 1$  for methane. Also, we choose the approximation [2], as the thermobaric relation (7):

$$T = A\ln P + B, \ A > 0, \ B > 0$$

or

$$T = A \ln \left( P/P_0 \right), \ P_0 = e^{-B/A} > 0.$$

Then the dependence of gas density on pressure

$$\rho_q = P / \left[ A R \ln \left( P / P_0 \right) \right]$$

has the form shown in Fig.4, and we can limit the range  $eP_0 << P_i < P_a < P_2|_{\psi_{\rho}=0}$ in determining the iterative solution for (37), (38), (39).

There are  $\rho_{g0} = \rho_g|_{\psi_{\rho}=0}$ ,  $P_1 = P_1|_{\psi_{\rho}=0}$ ,  $P_2 = P_2|_{\psi_{\rho}=0}$ ,  $\rho_{g\min} = eP_0/(A R) < \rho_g|_{\psi_{\rho}=0}$  in Fig.4.



FIGURE 4. The dependence of gas density on pressure.

**5.2. Two-phase equilibrium in the thawed zone.** Similar to Section 5.1, the balance equations have the form (we assume  $S_{\nu} = 1$ ):

(41) 
$$m\left[S_w\rho_w\right] = M_w,$$

(42) 
$$m\left[(1-S_w)\rho_g\right] = M_g$$

(43) 
$$m \left[ S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \varepsilon_g \right] + (1 - m) \rho_s \varepsilon_s = E.$$

Since  $S_{\nu} = 1$ , then  $\psi_h = 0$  follows from (40), i.e.:

$$-(m\rho_w - M_w)\rho_g + M_g\rho_w, \ (m\rho_w - M_w) > 0.$$

In addition, from (37) it follows:

$$-\Phi_p + \frac{1}{T} \left[ P + E \right] = 0.$$

Here  $\Phi_p > 0$  according to (36).

Some initial approximation  $P_*$  is given for nonideal gas  $(z_g \neq 1 \text{ in } (12))$  in the iterative process (44) by definition of pressure P.

(44) 
$$\frac{P}{z_g(P,T) R T} = \frac{M_g \rho_w}{m \rho_w - M_w}, \ T = \frac{P + E}{\Phi_p}$$

The following relations can be used to determine the thermodynamic parameters P and T in the case of an ideal gas ( $z_g = 1$  in (12)):

(45) 
$$\frac{E}{P} = \frac{(m\rho_w - M_w)}{M_g \rho_w} \frac{\Phi_p}{R} - 1, \ T = \frac{P + E}{\Phi_p}.$$

Further, the water saturation  $S_w$  is determined by taking into account (41).

**5.3. Double skeleton.** We choose a value  $\Delta_{\nu} < 1$  close to one. We fix the closeto-unit thaw  $S_{\nu} \to 1$ , such that  $\Delta_{\nu} < S_{\nu} < 1$ , as a parameter in this node  $\omega$ . In the physical sense, we produce the hydrated encapsulation in the node balance domain  $d(\omega)$  of the grid, i.e. we suppose that the new solid skeleton of the system (labeled with an index k) consists of two parts: the old skeleton with a density  $\rho_s$ , the volume fraction of which is in space (1-m) and the encapsulated hydrate with density  $\rho_{\nu}$  and volume fraction  $(m-m_{\nu})$ . Here  $m_{\nu} = m S_{\nu}$  is interpreted as the encapsulated porosity of the two-phase system, i.e. that fraction of the volume in which the flow of free fluids (water and gas) occurs. Thus, we can write for the density of the framework, for its internal energy and enthalpy per unit mass:

(46) 
$$\rho_k = \frac{m - m_\nu}{1 - m_\nu} \rho_\nu + \frac{1 - m}{1 - m_\nu} \rho_s,$$

(47) 
$$\varepsilon_k = \frac{1}{\rho_k} \left[ \frac{m - m_\nu}{1 - m_\nu} \rho_\nu \varepsilon_\nu + \frac{1 - m}{1 - m_\nu} \rho_s \varepsilon_s \right],$$

(48) 
$$i_k = \varepsilon_k + \frac{P}{\rho_k}$$

Here

(49) 
$$i_k = f_{pk} T - \frac{m - m_\nu}{1 - m_\nu} \frac{\rho_\nu}{\rho_k} h,$$

(50) 
$$f_{pk} = \frac{1}{\rho_k} \left\{ \frac{m - m_\nu}{1 - m_\nu} \rho_\nu (\beta_w \, c_{pw} + (1 - \beta_w) \, c_{pg} + \frac{1 - m}{1 - m_\nu} \, \rho_s \, c_{ps}) \right\}.$$

Here  $f_{pk}$  is the frame that capacity of a unit mass at constant pressure.

We write instead of the masses  $M_w$  and  $M_g$  (see the beginning of Section 5), the part of them that falls on the flow of free water and gas and corresponds to the encapsulated porosity  $m_{\nu} = m S_{\nu}$ :

(51) 
$$M_{\nu w} = M_w - m(1 - S_{\nu})\beta_w \rho_{\nu},$$

(52) 
$$M_{\nu g} = M_g - m(1 - S_{\nu})(1 - \beta_w)\rho_{\nu}.$$

Then we rewrite the system (33),(34),(35):

(53) 
$$m_{\nu} \left[ S_w \rho_w \right] = M_{\nu w},$$

(54) 
$$m_{\nu} \left[ (1 - S_w) \rho_g \right] = M_{\nu g},$$

(55) 
$$m_{\nu} \left[ S_w \rho_w \varepsilon_w + (1 - S_w) \rho_g \varepsilon_g \right] + (1 - m_{\nu}) \rho_k \varepsilon_k = E.$$

It coincides with the system of equations (41),(42),(43) for a two-phase equilibrium thawed zone with a formal replacement:

(56) 
$$m_{\nu} \leftrightarrow m, \ M_{\nu w} \leftrightarrow M_{w}, \ M_{\nu g} \leftrightarrow M_{g}, \ \rho_{k} \leftrightarrow \rho_{s}, \ \varepsilon_{k} \leftrightarrow \varepsilon_{s}.$$

The enthalpy ratio follows from (55):

(57) 
$$m_{\nu} \left[ S_w \rho_w i_w + (1 - S_w) \rho_g i_g \right] + (1 - m_{\nu}) \rho_k i_k = E + P.$$

Thus, we can switch the calculation mode from the three-phase hydrate-containing state to the two-phase thawed zone with a double skeleton by recalculating the form (56) in separate node-balanced domains  $d(\omega)$  of the difference grid. Moreover, the double skeleton can be interpreted as a medium with a simple skeleton. And the reverse transitions from the two-phase thawed zone (with double skeleton or simple skeleton) to the three-phase hydrate-containing state are also possible.

**5.4. Evolutionary Transphase Algorithms.** The information presented in the previous sections allows us to suggest some regularization methods for evolutionary transphase calculations of joint filtering problems in a piezoconductive medium with gas hydrate inclusions and in the thawed free hydrate zone, with preserving the complete conservatism of the corresponding difference algorithms.

5.4.1. Double skeleton method. The transition from a three-phase medium with gas hydrate inclusions to a two-phase thawed hydrate free zone using the double skeleton method (see Section 5.3) at this time step is used as one of the possible types of regularization of transphase calculations. Later, the double skeleton is transformed into a simple skeleton in subsequent time steps, if the system has enough energy in the node balance domain  $d(\omega)$  to remain two-phase (Section 5.2). That, the condition  $T \geq T_{dis}$  is fulfilled. Or the system finds its thermodynamic equilibrium as a three-phase hydrate-containing medium (Section 5.1) if its temperature is below the dissociation temperature  $T_{dis}$  (see (7)).

5.4.2. Overheated thaw method. Overheated thaw with a balanced transition to a two-phase thawed zone with a simple skeleton is as follows. If a three-phase medium with gas-hydrate inclusions was calculated in the node balance domain  $d(\omega)$  and the thaw  $S_{\nu}$  exceeded a unit value  $(S_{\nu} \geq 1)$ , this means that three-phase thermodynamic equilibrium determined by the parameters  $M_w$ ,  $M_g$ , E according to (33),(34),(35) does not exist. Since the thermodynamic equilibrium state of the medium is determined uniquely, then the solution  $\{S_w, P, T\}$  corresponding to the thermodynamic equilibrium two-phase thawed zone according to (41),(42),(43) is determined by the same parameters  $(M_w, M_g \text{ and } E)$ . The subsequent calculation in this node  $\omega$  in subsequent time steps occurs already in the two-phase thawed zone with a simple skeleton.

5.4.3. Supercooled thawed zone method. We calculate the two-phase thawed zone in the node balance domain  $d(\omega)$  (with a simple skeleton or a double skeleton) and the temperature is below the dissociation temperature (i.e.  $T < T_{dis} = f(P)$ , see (7)) at this time step in the node  $\omega$ . Then, we use the values  $\{M_w, M_g \text{ and } E\}$  known from (41),(42),(43) in the thawed zone and we calculate  $\{S_{\nu}, S_w, P\}$  and  $T\}$  according to (33),(34),(35) for the three-phase hydrate-containing state. Further calculation in this node  $\omega$  in subsequent time steps occurs in the three-phase hydrate-containing zone. It is possible to modify this approach, if the condition  $T < T_{dis}$  is fulfill in this node  $\omega$ , then the recalculation according to equations (33),(34),(35) is not performed and the three-phase hydrate-containing state on an explicit time layer is  $S_{\nu} = 1$  and the values  $S_w$ , P and T from the thawed zone are known. In this case, the thermobaric condition (7) for the three-phase calculation is performed only at an implicit time step.

## 6. Results of calculations

6.1. Numerical modeling of one-dimensional problems of dissociation of gas hydrates in a porous medium. We consider the following spatial onedimensional process in the interval  $x \in [0, l]$ , l is the length of the calculated area. In it at the initial instant of time, three-phase equilibrium is observed, including a volumetric distributed solid hydrated phase. In this state of the system, the pressure  $P(x,0) = 3 \times 10^6$ Pa, water saturation  $S_w(x,0) = S_w^*$  and hydrate thaw  $S_{\nu}(x,0) = S_{\nu}^*$  are homogeneous in space in this system state,  $0 < S_w^* < 1$  and  $0 < S_{\nu}^* < 1$  are constant values. Acceleration of gravity is not taken into account (g = 0). The left boundary of the calculated area is impermeable solid "wall", i.e. the mass flow through it is zero:  $V_w|_{x=0} = 0$ ,  $V_g|_{x=0} = 0$ , t > 0. In this time the right boundary has depression pressure  $P(x, l) = 10^5$  Pa. Heat fluxes at the boundaries of the region are absent. Volumetric sources of mass and energy in the medium are also absent:  $q_w = 0$ ,  $q_q = 0$ ,  $q_{\varepsilon} = 0$ . Methane in the calculations is taken like ideal gas ( $z_g = 1$ ). The pressure dimension in the formulas of Section 5.1.1 was measured in pascals: [P] = Pa.

The parameters of the Messoyakha's gas hydrate deposit [9] were selected for simulation.

$$\begin{split} \rho_w &= 10^3 \frac{kg}{m^3}, \ \rho_\nu = 910 \frac{kg}{m^3}, \ \rho_s = 2800 \frac{kg}{m^3}, \ \beta_w = 0.9, \ m = 0.35, \ A = 7.28K, \\ B &= 169.7K, \ \mu_w = 10^{-3} Pa \cdot s, \ \mu_g = 0.014 \cdot 10^{-3} Pa \cdot s, \\ c_{pw} &= 4200 \frac{J}{kg \cdot K}, \ c_{pg} = 2500 \frac{J}{kg \cdot K}, \ c_{ps} = 873 \frac{J}{kg \cdot K}, \ M = 0.016 \frac{kg}{mole}, \\ h &= 514810 \frac{J}{kg}, \ R = 8.31 \frac{J}{mole \cdot K}, \ S_w^* = 0.6, \ S_\nu^* = 0.75, \ k(S_\nu) = k_0 \cdot (S_\nu)^3, \\ k_0 &= 10mD = 10^{-14}m^2, \ k_{rw}(S_w) = 1.477S_w^5 - 1.587S_w^6 + 1.11S_w^7 - 0.0473, \\ k_{rg}(S_w) &= 1.044 - 1.7S_w + 0.6S_w^2 \end{split}$$

The minimum value of water saturation is  $S_{w \min} = 0.55$ .

$$k_{rw}(S_w) = 0, \ k_{rg}(S_w) = k_{rg}(S_{w\min}) \ at \ S_w \le S_{w\min}.$$

The maximum value of water saturation is  $S_{w \max} = 0.9$ .

$$k_{rw}(S_w) = k_{rw}(S_{w\max}), \ k_{rg}(S_w) = 0 \ at \ S_w \ge S_{w\max}.$$

The thermal conductivity of the medium was taken into account according to formulas (6) and (20) and was taken equal to  $\lambda_w = 0.561$ ,  $\lambda_g = 0.0342$ ,  $\lambda_\nu = 2.11$ ,  $\lambda_s = 0.2 \frac{W}{m \cdot K}$ . The length of the model area was assumed to be equal to l = 1 m, a step in the

The length of the model area was assumed to be equal to l = 1 m, a step in the space coordinate was h = 0.01 m. Calculations were carried out for time moments t = 500, 1000, 2000, 6000, 12000 s.

In Fig.5, 6, 7, 8, 9, 10, we can see that in the calculations a joint transphase process of volumetric phase transitions of the medium in the emerging thawed zone and in the rest of the collector piezoconductive medium with gas hydrate inclusions is implemented. This process expands spatially from right to left inside the zone of depression. Such transphase calculations, in particular, make it possible to study local processes of technogenic depressive effects directly in the vicinity of wells on the dynamics of the spatial distributions of gas hydrates thaw and the formation of thawed two-phase zones.



FIGURE 5. The distribution of hydrate thaw for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s. Two phase thawed zone on the right is highlighted in red.



FIGURE 6. The distribution of water saturation for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s. Two phase thawed zone on the right is highlighted in red.



FIGURE 7. The distribution of pressure for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s. Two phase thawed zone on the right is highlighted in red.



FIGURE 8. The distribution of temperature for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s. Two phase thawed zone on the right is highlighted in red.

The pressure graphs (see Fig.7) show that the presence of water saturation and hydrate thaw has little effect on the nature of the pressure distribution, and it changes almost as in the one-phase case. At a developed stage of the process, the pressure tends to be constant, and, accordingly, the velocities of gas and water filtration, proportional to the pressure gradient, and the divergent terms of the equations in the thawed zone (17), (18), (19) depending on them also tend to zero.



FIGURE 9. The temperature dependence on pressure in the whole plane P, T for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s.



FIGURE 10. The temperature dependence on pressure in the zone of violation of three-phase thermobaric equilibrium  $T_{dis} = f(P)$  with the transition to the thawed zone for moments of time 500, 1000, 2000, 6000, 9000 and 12000 s.

Thus, the solution is stabilized, and the system of equations takes the form (41), (42), (43). The values of water saturation and temperature determined in this case are found from the stabilization of solutions of the non-stationary problem.

In the substantial absence of filtration at the final stage of the process, the residual temperature dynamics (fractions of a degree) is determined by the thermal conductivity.

From a comparison of the graphs  $S_{\nu}(x)$ , T(x) (see Fig. 5, 8) for the same times t, we can see the transition from the three-phase zone, where the pressure and temperature are related by the formulas of Section 5.1.1 to the two-phase zone, where the process flows almost isothermally, which corresponds to the assumptions made in most cases that the two-phase filtration is isothermal.

This is confirmed by the graphs of the dependence T(P) (see Fig. 9,10), where two characteristic regions are visible, corresponding to the three-phase and twophase zones. Of further interest is the development of algorithms for the joint calculation of three-phase hydrate-containing states and two-phase systems from hydrate and free gas or water, as well as a generalization of the results obtained in the case of the introduction of volume fractions of water and ice in the phase equilibrium zone.

6.2. Spatial-three-dimensional calculations of piezoconductive processes in a three-phase hydrate-containing medium near the depression craters of wells. In order to demonstrate the capabilities of the proposed technique, the final section presents the solution of model three-dimensional problems with depression funnels near the wells of the piezoconductivity equation (14), (16) in a three-phase medium with hydration inclusions with fixed saturation value  $S_{\mu}^{*}$  and  $S_w^*$  (see also Section 4.1). In contrast to section 6.1, a spatial three-dimensional cube is considered. In it, at the initial moment of time, a three-phase equilibrium is observed, which includes the solid-hydrated phase, which is volume-distributed. In this state, the pressure was taken  $P = 7.4 \times 10^6$  Pa, while the depression pressure in the wells was considered equal to the atmospheric pressure of  $-10^5$  Pa. Water saturation  $S_w = 0.6$  and thaving  $S_{\nu} = 0.75$  are homogeneous in space and do not change. The acceleration due to gravity is not taken into account (q = 0). All walls of the computational domain are also assumed to be leaky. Heat flows at the borders of the region are also absent. In calculations, methane gas was taken as an ideal  $(z_q = 1)$ , the pressure dimension in the formulas of section 5.1.1 measured in Pascals: [P] = Pa. The remaining values of the physical parameters are similar to those presented in Section 6.1.

Two tasks were solved: for one downhole well and for the development zone from several well clusters. All tasks were considered in a three-dimensional setting, the score was kept on establishment. The size of a cylindrical well was  $1 \times 20$  m. All grids in the calculations are tetrahedral, thickening to the peculiarities of the computational domain (wells).

Task 1. Study of one downhole. The size of the area is  $500 \times 500 \times 500$  m<sup>3</sup>. The grid consists of 378,200 elements (Fig. 11). The volume distribution of pressure, as well as pressure and temperature profiles are presented in Fig. 12, 13.



FIGURE 11. Calculation grid for modeling of one depression funnel.

For clarity, the depression funnel formed in the area of the well is shown upside down.

Task 2. Modeling the development zone of two well clusters. The size of the area is  $2000 \times 2000 \times 2000$  m<sup>3</sup>. The distance between the wells is about 100 m, between the bushes -1 km. The size of the grid - 2114202 elements. The grid and volume distribution of pressure are presented in Figures 14 and 15.

Figure 15 shows several types of pressure distribution in the central development zone with different scales in order to more clearly show the effect of the central part



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FIGURE 14. Calculation grid for modeling the central zone.

of the zone. It is seen that separately standing bushes of wells interact with each other, thereby forming extended areas of depression.

The three-dimensional calculations of the piezoconductive-dissipative block of equations (14), (16) show the typical pattern of pressure distribution in the bottomhole zones and in the reservoir and do not contradict the actual situation that occurs during the development of the field. Problems are solved in the case of three-phase volume equilibrium of water, free gas and hydrates.

## 7. Conclusion

A mathematical model has been developed that allows to investigate numerically the fluid dynamics in a porous medium within the framework of a single scheme, taking into account gas hydrates both in the three-phase zone and in the thawed zone containing only gas and water. The computer programs based on this model for a one-dimensional case (linear and radial) are created. Difference schemes based on the support operator method are constructed for solving problems of this type in the non-one-dimensional case. The applicability of the support operator method is shown for a unified description of fluid-dynamic and deformation processes in a porous medium with allowance for gas hydrates. The method used in the work



FIGURE 15. Volumetric pressure distribution of the central development area: various types.

is based on the splitting of water and hydrate saturation transfer by the physical processes, on the one hand, and the separation of piezoconductive processes that take into account the presence of a solid hydrate phase in the pores, on the other hand. The algorithms are written and the program implementation is developed. A joint transphase calculation was performed with time-varying spatial localizations of different numbers of phases. The results of calculations show the effectiveness of the developed methods for calculating real problems associated with gas hydrates deposits. They also show the effectiveness of the developed methods for the study of complex transphase processes, as well as the dynamics of water and hydrate saturation in the reservoir.

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