Simulation of deformation and fracture of fluid-saturated porous media with hybrid cellular automaton method

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Abstract

In the paper we propose the method of numerical simulation of fluid-saturated porous media, that represents the combination of particle method and finite-difference method, namely hybrid cellular automaton method. It allows explicit taking into the account inelastic deformation, dilation and fracture of solid skeleton as well as the influence of pore pressure on the stress state of the skeleton and the redistribution of a fluid in filtration volume of porous medium. We applied the method to study the influence of viscous compressible liquid in pores of material to its strength and fracture. It has been shown that the influence of the liquid in pores significantly depends on elastic-plastic properties of material of solid skeleton.

Keywords: Porous medium, fluid, inelastic deformation, fracture, strength, numerical simulation, MCA method, finite-difference method.

1. Introduction

Porous media, saturated with a fluid, represent a wide class of physical and biological objects, like a geological media, including coal seams, oil vessels etc, a biological media, such as a bone tissue, and a technical objects of a different purpose, including filtering materials, endoprostheses etc (Zhejun (2007), Taylor (2007), Zavsek et al

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At that, the study of a response of such media to mechanical loading, including their deformation and fracture, remains the problem of high importance. In the paper we propose the method of theoretical study of fluid-saturated porous media, namely the hybrid cellular automaton method, and the results of its application to investigation of a features of fracture elastic-plastic and brittle specimens, filled with liquid.

2. Keystones of hybrid cellular automaton method

Let us consider a medium that consists of a solid skeleton and a system of pores of different scales, filled with liquid. The problem of description of this medium splits into two inter-connected problems: 1) description of mechanical behavior of solid skeleton and 2) description of transfer of a fluid in pore volume. In the framework of the proposed approach, we use the movable cellular automaton (MCA) method (Psakhie et al (2013)) to simulate a deformation and fracture of a solid skeleton and the finite-difference mesh (FDM) to simulate a mass transfer of a fluid. These layers, constructed by MCA and FDM, are interconnected together by means of projection of properties of a solid skeleton from MCA to FDM and backward projection of pressure of a fluid from FDM to MCA layer (Fig. 1a). In the framework of proposed method spatial motion and rotation of movable cellular automata leads to transfer of properties (including pressure of a fluid, its concentration etc) of nodes of FDM, belonging to corresponding movable cellular automata (Fig.1b). This results in the explicit taking into the account of motion of elements of a solid skeleton when modeling the transport of a fluid on FDM. The computational accuracy of this approach is determined by the ratio of the size of movable cellular automaton to the size of a cell of FDM – the greater this ratio, the more precise is the approach.

2.1. Keystones of movable cellular automaton method

The movable cellular automaton method represents the particles method, formulated as a discrete elements method (Psakhie et al (2013)). In the framework of MCA method we use the principle of multiparticle interaction to describe the forces acting between discrete elements. This approach allows adequate implementation of a variety of rheological models of solids, including multi-parametric models of plasticity (Psakhie et al (2011)).

![Fig. 1. The layers of movable cellular automaton and finite-difference mesh (a); the transfer of properties of nodes of finite-difference mesh as the result of displacement and rotation of movable cellular automaton.](image)

In the framework of MCA method the mechanical response of elastic-plastic material is described within the model of plasticity with non-associated flow law and von Mises yield criterion, also known as Nikolaevsky model (Garagash, Nikolaevsky (1989)). This model postulates the linear dependence between shear strain rate and volumetric strain rate. Mentioned approach allows adequate description of a mechanical response of materials with dilatational plasticity, including the accounting of contributions of underlying scale levels. The Nikolaevsky model of plasticity has been implemented on the basis of Wilkins algorithm, that reduces the solution of elastic-plastic problem to the solution on an elastic problem with consequent correction of interaction forces between particles in such a way to keep a value of local pressure constant (Wilkins (1999)). An elastic interaction between pair of \(i\)-th and \(j\)-th movable automata is defined on the basis of the generalized Hooke's law in hypoelastic form (Stefanov, (2002)):
\[
\begin{align*}
\Delta \sigma_{ij} &= \Delta \sigma_{ij}^\text{center} / S_{ij} = 2G_i (\Delta e_{ij} - \Delta P^\text{fluid}_i / K_i) + (1 - 2G_i / K_i) \Delta \bar{\sigma}_i^\text{mean}, \\
\Delta \tau_{ij} &= \Delta \tau_{ij}^\text{tang} / S_{ij} = 2G_i \Delta \gamma_{ij}^\text{int},
\end{align*}
\]

where symbol \( \Delta \) denotes an increment of a value of corresponding parameter during a time step; \( \sigma_{ij} \) and \( \tau_{ij} \) – specific values of axial (\( F_{ij}^\text{center} \)) and tangential (\( F_{ij}^\text{tang} \)) components of interaction force between \( i \)-th and \( j \)-th elements; \( S_{ij} \) – contact area between \( i \)-th and \( j \)-th elements; \( G_i \) and \( K_i \) – shear and bulk modules of a material of \( i \)-th element; \( \Delta e_{ij} \) and \( \Delta \gamma_{ij}^\text{int} \) – increments of axial and tangential deformations of \( i \)-th element in \( i-j \) pair; \( \bar{\sigma}_i^\text{mean} \) – mean stress in the volume of \( i \)-th element; \( P^\text{fluid}_i \) – contribution of the pore pressure of a fluid into mean stress in the volume of \( i \)-th element. Mean stress \( \bar{\sigma}_i^\text{mean} \) is calculated on the basis of Love’s relation, which states the connection between components of stress tensor (\( \sigma_{ij} \)), defined in given volume, and forces, acting on the surface of this volume (Psakhie et al (2013)). Note that in the framework of the developed model we assume that the pressure of fluid \( P^\text{fluid}_i \) contributes only into the value of hydrostatic stress in solid skeleton (hydrostatic tension). This assumption is adequate under the absence of specific geometry and orientation (texture) of porosity.

The yield stress criterion, which takes into the account the contribution of porous pressure of a fluid, is formulated in the following form:

\[
\Phi_i = \beta_i (\bar{\sigma}_i^\text{mean} + P^\text{fluid}_i) + \sqrt{3} \gamma_i > Y_i,
\]

where \( Y_i \) – is shear yield strength of a material of \( i \)-th element, \( \beta_i \) – coefficient of internal friction, \( \gamma_i^\text{int} \) – von Mises stress (in the volume of \( i \)-th element).

Scaling (returning) of the components of stress deviator is performed by the following way (Wilkins (1999)):

\[
\begin{align*}
\sigma'_{ij} &= (\sigma_{ij} - \bar{\sigma}_i^\text{mean}) M_i + (\bar{\sigma}_i^\text{mean} - N_i) \\
\tau'_{ij} &= \tau_{ij} M_i
\end{align*}
\]

where \( (\sigma'_{ij}, \tau'_{ij}) \) – are corrected specific values of axial and tangential reaction forces; \( M_i = 1 - \sqrt{3} / \sqrt{\bar{\sigma}_i^\text{int}} (3G_i (\Phi_i - \gamma_i^\text{int}/(K_i \Lambda_i \beta_i + G_i)) - \text{is the correction coefficient derived from the algorithm of Wilkins}; \( N_i = K_i \Lambda_i (\Phi_i - \gamma_i^\text{int}/(K_i \Lambda_i \beta_i + G_i) - \text{is the correction of the value of mean stress}; \( \Lambda_i \) – coefficient of dilation of material of \( i \)-th element.

In the framework of the model we use the modified Drucker-Prager criterion as the criterion of failure (i.e. loss of the linkage between particles):

\[
\sigma_{DP} = 0.5(a + 1)\sigma_{\text{in}} + 1.5(a - 1)(\bar{\sigma}_{\text{mean}} + P^\text{fluid}_i) > \sigma_c,
\]

where \( \sigma_c \) – ultimate strength for a given pair of elements, \( \sigma_c \) and \( \sigma_t \) – compression and tensile strengths of a link between given pair of elements, \( a = \sigma_c / \sigma_t \).

2.2. Simulation of transfer of liquid within finite-difference mesh

In the framework of the developed model of transfer of liquid we take into the account the multi-level structure of porous skeleton by means of introducing of integral parameters of structure from lower scales, namely the value of open porosity (filtration volume), represented by a system of pores and channels in the bulk of material, interconnected with each other and with the surface. At that, we use the following assumptions: 1) a liquid can
occupy as pore volume as a whole, as partially; 2) adsorption of a liquid on a surfaces and capillary effects are not taken into account; 3) a liquid is compressible. We use the following state equation of liquid:

\[ \rho(P) = \rho_0 \left(1 + \frac{(P - P_0)}{K_{\text{liq}}} \right), \]  

(5)

where \( K_{\text{liq}} \) – compression modulus of a liquid, \( \rho \) – density of a liquid, \( P \) – pressure, \( \rho_0 \) and \( P_0 \) – values of density and pressure of a liquid at atmospheric conditions.

In the framework of the developed model, we simulate the transfer of a density of a liquid under the influence of gradient of pressure of a liquid, that is the driving force of filtration. The equation of transfer of a density is based on Leibenzon equation (Basniev et al., (2012)):

\[ \gamma_{\text{open}} \frac{\partial \rho}{\partial t} = K_{\text{liq}} \left[ \frac{k}{\eta} \nabla \rho \right]. \]

(6)

where \( \gamma_{\text{open}} \) – open porosity, \( \eta \) – viscosity of the liquid, \( k \) – coefficient of permeability of solid skeleton, that can be defined as follows: \( k = \gamma_{\text{open}} d_{ch}^2 \), where \( d_{ch} \) is the characteristic diameter of filtration channels. The numerical integration of (6) is carried out using the alternating direction implicit method.

The main feature of a liquid, in comparison with gaseous one, is the possibility of a partial filling of a pore volume (while a gas fills the whole free volume). When a liquid fills a pore volume partially, the pressure of a liquid skeleton can be assumed equal to zero (at the same time, a pressure of a gaseous fluid is always greater than zero). Correspondingly, in order to adequately describe a transfer of a liquid it is necessary to develop the special mathematical formalism. As it was told above, a liquid can occupy a volume smaller that a whole vacant volume of a pore. Correspondingly, at \( \rho \leq \rho_0 \) the pressure of a liquid will be equal to \( P = P_0 \). In the framework of used assumptions, there is no mass transfer of a liquid between nodes of finite-difference mesh, if \( \rho \leq \rho_0 \) in both nodes.

2.3. The interconnection between movable cellular automaton and finite-difference mesh

In the framework of proposed hybrid cellular automaton method a solid skeleton and a fluid are considered as interconnected systems. The influence of pore pressure of a fluid \( P_i^{\text{fluid}} \) on an ensemble of movable cellular automata is performed by means of including the value of \( P_i^{\text{fluid}} \) into equations (1), (2) and (4). The pore pressure \( P_i^{\text{fluid}} \) is defined as follows: \( P_i^{\text{fluid}} = P_i^{\text{open}} \gamma_i^{\text{open}} \), where \( P_i^{\text{open}} \) – averaged pore pressure in open porosity, within the assumption of uniform distribution of pores, cracks and filtration channels in a solid skeleton, without a respect to their geometry and orientation. The pressure \( P_i^{\text{open}} \) is determined by means of averaging of corresponding pressures in nodes of finite-difference mesh, related to \( i \)-th movable cellular automaton.

The mechanical stresses in a solid skeleton lead to a changes in volume of open porosity, that, in turn, leads to a change of pressure of a fluid. The relation between porosity and mechanical stresses in a solid skeleton is described as follows:

\[ \gamma_i^{\text{open}} = \gamma_i^{\text{init}} (1 + \Omega_{\text{elast}}) + \Omega_{\text{plast}}, \]

(7)

where \( \gamma_i^{\text{init}} \) is initial value of open porosity, \( \Omega_{\text{elast}} \) and \( \Omega_{\text{plast}} \) – local values of elastic and plastic deformations:

\[
\begin{align*}
\Omega_{\text{elast}} &= \frac{3(\sigma_{\text{mean}} + P_i^{\text{fluid}})}{K}, \\
\Omega_{\text{plast}} &= \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} - \Omega_{\text{elast}}.
\end{align*}
\]

(8)

Equations (1), (2), (4), (7)- (8) describe the interference between models of a solid skeleton and a fluid, which are implemented in the framework of the hybrid cellular automaton method.
3. Influence of fluid on the response of porous specimens

The developed model has been applied to the simulation of uni-axial loading of porous specimens, filled with water. The specimens were mounted between immovable supporting plate from below and piston from above (Fig. 2a). The piston moved downwards with constant velocity of 0.01 m/sec. The problem was solved in two-dimensional formulation in the approximation of plane stress state. It was assumed that a fluid is absent in the outer space of a specimen. The coefficient of dilatancy was \( \lambda = 0.173 \), the coefficient of internal friction was \( \beta = 0.49 \). The structure of specimens was assumed to be uniform; there were no macroscopic pores and inclusions. The peculiarities of the mechanical response of the specimens of brittle and elastic-plastic (with properties close to sandstone) materials has been studied (stress-strain diagrams for a mechanical response of a pair of movable automata are shown in Fig. 2b).

It was revealed that a pore pressure of a liquid plays a significant role for a mechanical response of brittle porous specimens. The fracture in these specimens is realized, as a rule, by means of nucleation and drastic growth of macroscopic crack, at that, a quasi-plastic response and corresponding dilation effects are negligible. During loading, the pore pressure of a liquid in brittle porous specimens increases until failure of the specimen and, thereby, influence on strength and deformation capacity. The dependence of compression strength of water-saturated porous brittle material on pore pressure is shown in Fig. 3a. One can see the decrease of strength of samples under increase of pore pressure of water. At that, the rate of decrease of strength depends on the value of open porosity.

The behavior of the elastic-plastic porous specimens, saturated with water, is significantly different from the above-described behavior of brittle specimens. In Fig. 3b one can see the dependencies of axial stress and pore pressure of water on axial deformation of specimens under uni-axial loading. Geometry of specimens and boundary conditions corresponded to those used in previous tests, porosity of material was \( \gamma = 10\% \). The initial pressures of water in pores were equal to zero and to 5 MPa (that corresponds to seam pressure at a depth of 500 meters). As it is shown in Fig. 3b, at the stage of elastic response (graph area I) the pore pressure of water linearly increases as the volume of open porosity linearly decreases. As the stage of inelastic deformation begins (graph area II), discontinuities of a different scales and dilation of material appear. As the result, the specific volume of voids in the solid skeleton increases, that leads in rapid drop of pressure of water down to zero. Thus, at the stage of inelastic deformation the porous water-filled specimen behaves equally to a "dry" specimen. This fact causes the observed weak dependence of strength of elastic-plastic materials on an initial pressure of water.

The results above demonstrate the fact, that pressure of a fluid in pore volume doesn’t play a determining role in the influence of a fluid on strength of elastic-plastic porous materials. So, we can suggest, that well-known experimental effect of decrease of strength in the presence of a liquid is conditioned by another physical mechanism (for example, Rebinder effect (Rebinder, Shchukin, 1973)).

Fig. 2. Scheme of loading of the simulated specimen (a); mechanical properties of simulated materials.
Conclusions

In the paper we describe the developed approach to simulation of a fluid-saturated porous material. This approach, called the hybrid cellular automaton method, combines the movable cellular automaton method with finite-difference method. The proposed approach allows explicit taking into the account as deformation and fracture of a solid skeleton as mass transfer of a fluid in pore volume.

It was shown that a liquid in pore volume produces dramatically different influence on the mechanical response of brittle and elastic-plastic porous bodies. The condition of the absence of influence of a liquid on the strength of elastic-plastic solid skeleton is the presence of dilatation of the material under loading. Macroscopic dilatation of a material is the result of increase in volume of voids (including pores, micro-cracks etc), that, in turn, leads to decrease in pore pressure of a liquid and neglects its influence on strength of a specimen.

Acknowledgements

The study has been carried out within the SB RAS Program III.23.1.4 for Basic Research.

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