Rheological aspects of underground fluid dynamics and mass exchange processes

Maxim KHRAMCHENKOV ▪ Kazan Federal University ▪ mkhramch@gmail.com
Eduard KHRAMCHENKOV ▪ Scientific Research Institute of System Analysis of the Russian Academy of Sciences ▪ ekhramch@gmail.com

Érkezett: 2015. 10. 27. ▪ Received: 27. 10. 2016. ▪ http://dx.doi.org/10.14382/epitoanyag-jsbcm.2016.6

Abstract

Mechanics of porous media has theoretical basis provided by scientific disciplines such as rock mechanics, soil physics and so on. In the current knowledge, some complex processes in the geo-systems lack full theoretical description. The example of such processes is metamorphosis of rocks, filtration process in swelling soils, earthquakes and correspondent variations of stress-strain state. Chemical transformation of solid and fluid components, heat release and absorption, phase transitions, rock destruction occurs in such processes. Extensive use of computational resources in scope of traditional models of the mechanics of porous media cannot guarantee full accuracy of obtained models and results. In this work complete description of processes of mass exchange between fluid and poly-mineral materials in porous media from various kinds of rocks (primarily sedimentary rocks) have been examined. It was shown that in some important cases there is a storage equation of non-linear diffusion equation type. In addition, process of filtration in non-swelling soils, swelling porous rocks and coupled process of consolidation and chemical interaction between fluid and granulated materials are considered. In the latter case equations of physical-chemical mechanics of conservation of mass for fluid and granulated material are used. Rheological properties of different kinds of rocks are described.

Keywords: rock mechanics, mass exchange, stress-strain state, rheological correlations

Maxim KHRAMCHENKOV
is a full professor of Kazan Federal University. Doctor of Science (D.Sc., habilitate) in Mathematical Simulation, KSTU, Russia (2003) Scientific interest: thermal, hydraulic, mechanical and chemical processes in geo-systems, medicine and engineering.

Eduard KHRAMCHENKOV
is a senior researcher in Scientific Research Institute of System Analysis of the Russian Academy of Sciences. In 2008 defended his PhD thesis. Main scientific interests: Applied mathematics, mathematical simulation, biomechanics and hydrogeomechanics, coupled processes, numerical methods, C/C++, GPGPU computing, CUDA, OpenCL, OpenMP, MPI.

1. Introduction

Several complex processes in the geo-systems still lack full theoretical description. The examples of such processes are metamorphosis of rocks (rock metamorphism process), different oil discovery/recovery processes, magma intrusion processes, where chemical transformation of solid and fluid components occurs with non-linear variation of fluid pressure and correspondent variations of stress-strain state. We start with the analysis of metamorphosis process. Metamorphosis process is the global process that began instantaneously with the appearance of Earth and continues in modern time. There are two types of metamorphosis: dynamic metamorphism that takes place due to impacts and sharp changes of stress-strain state (*Fig. 1*), and contact metamorphism that takes place on contacts between hot magma intrusion and environmental rocks (*Fig. 2*). In case of large contact area of magma intrusion and environments the term regional metamorphism is used.

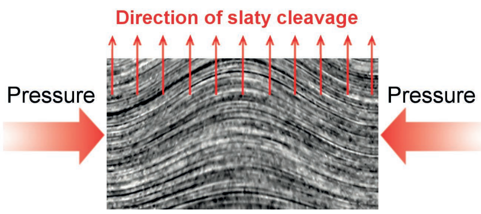

Fig. 1. Sketch of dynamic metamorphism
1. ábra Dinamikus metamorfózis vázlata

Metamorphism can take place in any kind of rock. We will analyze primarily the metamorphism of sedimentary rocks. Metamorphism of sedimentary rocks conducts through two stages: hydration and dehydration of rocks. The point is that metamorphism process connects with chemical and phase transformation of minerals, but we always can allot two these stages for any scenario of mineral transformation. Metamorphic dehydration is concluded in rejection of water from mineral lattice during its transformation and usually accompanies rock consolidation process. The process of rocks consolidation which happens due to filtration of underground fluids is described in the scope of classic rock mechanics [1-4]. Main principles of description of complex coupled thermo-chemical processes in geological systems are also described in the cited reference works.

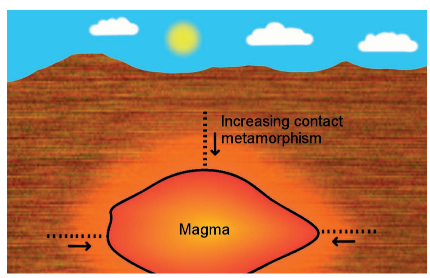

Fig. 2. Sketch of contact metamorphism
2. ábra Kontakt metamorfózis vázlata

Approaches to description of complex processes in geological systems, including chemical processes and interfacial mass transfer, are well-known and provided, for example, in [5]. But in these approaches one have to know equations of kinetics of chemical reactions in a system, which play role of closing relations of a system. Form of these relations is unknown in most of theoretically and practically interesting cases. Efforts that use some hypothetic forms lead to inaccuracies in results and thus conclusions on the basis of the results can be only approximate. We propose compromise between approximate estimations and physical realism in description of complex processes in geological systems. The metamorphic dehydration processes sometimes lead to the formation of sub-horizontal fluid systems. The main ideas and conclusions from [6] are summarized here in brief form:

- Metamorphic dehydration is the main source of fluids.
- Fluids influx from the upper mantle have subordinate value.
- Sub-horizontal parts of fluid systems are electro-conductive areas, wave conductors and areas of absorption of seismic waves.
- Sub-horizontal parts of fluid systems are large regulating storage-reactors.
- Fluids have great influence on the character of effective stresses and strength properties (balance between processes of compaction and decompaction).
- Deformation of fluid-saturated rocks and metamorphosis of rocks (when a fluid exudes due to dehydration) play the main role in formation of weakened fluid-saturated layer in middle parts of Earth crust.
- Metamorphic dehydration is the main factor of formation of seismically active layer, where the most of earthquake focuses are situated.

Processes of formation of hydro-carbonaceous fluids in clay sedimentary rocks can be examined on examples of Bazhenov-Abalak formation and sub-Achimov formation in Siberia, Russia [7]. The most important facts from the latter work are:

- Summary width of clays in Abalak, bituminous Bazhenov and sub-Achimov rock masses in the internal part of sedimentation basin is no less than 100-250 m.
- Filtrational-capacitative properties of Bazhenov clays are dictated by horizontal micro-fissuring. In case of Bazhenov formation term *fissuring* is relative, because these are not fissures in usual tectonic sense, but interstices of sheeting.
- There is an increase of clay density from the center of the rock mass to its roof and bottom. Clays in the center of the Bazhenov formation have densities not exceeding 1930 kg/m^3. In the roof and bottom parts of the formation densities are not less than 2400 kg/m^3. Clays with normal density that besiege the internal part of the Bazhenov formation have sealing properties that are usual for clays.
- Presence of overpressure in the internal part of formations; overpressure disappear near the roof and the bottom.

Intrusion of liquid magma into rocks with transformation of material of rocks and components of magmatic molten mass is another example of complex mass transfer in geological systems. In such cases characteristic intrusive forms appear (for example lopolith).

Effective equations of diffusion-reaction for concentrations are presented in [11]. This approach does not erase a problem of choice of precise form of kinetic equation. It is possible that choice of a new effective variable and derivation of a new governing equation for this variable is a better approach. In our approach we use volumetric deformation as an effective variable and it gives an opportunity to obtain uniform description both of deformations and chemical interactions.

2. System of basic differential equations

Let us consider the porous media consolidating under the weight of overlying rock with coupled complex geological processes, as a continuous porous medium of variable mass. There are a lot of components of underground fluid that take part in mass exchange reactions with corresponding components of solid phase of porous medium. Let the non-active components of solid phase have density of ρ_s and occupy volume V_s in representative volume of porous medium **V**. The equation of conservation of mass of the fluid is

$$\partial(mS\rho)/\partial t + \mathrm{div}(m\rho S\mathbf{V}) = -j \quad (1)$$

where m is porosity; S is the fluid saturation of pores; ρ is fluid density; **V** is the average velocity of the fluid; j is the exchange mass flux.

The equation of conservation of mass of the particles is

$$\partial[(1-m)\rho_s^f]/\partial t + \mathrm{div}[(1-m)\rho_s^f\mathbf{W}] = j \quad (2)$$

where ρ_s^f is the total density of the particles material; **W** is the average velocity of particles. The equation for solid phase mass M_s in the representative volume is

$$M_s = \rho_s V_s + \rho_a[(1-m)V - V_s],\ \ \rho_s V_s = M = \mathrm{const} \quad (3)$$

Here, ρ_s is the density of non-active solid phase material; ρ_a is the density of absorbed components of fluid.

The volume strain of the porous medium is

$$\theta = (V - V_0)/V_0 \quad (4)$$

where V_0 is the initial value of V. Usually θ is small and we can rewrite Eq. (4) as

$$V = V_0 \exp\theta,\ V_0 = V(\theta = 0). \quad (5)$$

Eq. (5) can be expressed by consecutive substitution from Eq. (3). The result is

$$M_s = M(1\text{-}\varepsilon) + \rho_a(1\text{-}m)V,\ \varepsilon = \rho_a/\rho_s.$$

It now follows that

$$\partial M_s/\partial t = -M\frac{\partial\varepsilon}{\partial t} + (1-m)V\partial\rho_a/\partial t + (1-m)\rho_a V\partial\theta/\partial t - \rho_a V\frac{\partial m}{\partial t}. \quad (6)$$

The total density of the particles material ρ_s^f and exchange mass flux j can be expressed as

$$\rho_s^f = \frac{M_s}{(1-m)V} = \rho_a + \frac{M(1-\varepsilon)}{(1-m)V},\ j = \frac{\partial M_s/\partial t}{V}.$$

It now follows, with Eq. (2), that

$$\partial\theta/\partial t = \mathrm{div}\mathbf{W}. \quad (7)$$

After some transformations the equation of conservation of mass of the fluid can now be expressed as

$$mS\rho^{-1}\partial\rho/\partial t + (1-m)\delta\rho_a^{-1}\partial\rho_a/\partial t + m\partial S/\partial t + \mathrm{div}\mathbf{q}$$
$$+[mS + \delta(1-m)]\partial\theta/\partial t = \frac{M}{\rho V}\frac{\partial\varepsilon}{\partial t} + (\delta - S)\frac{\partial m}{\partial t} \quad (8)$$

where $\rho_a/\rho = \delta$. The simplest situation is single-phase filtration for the case of low compressibility of fluid, absorbed phase and particles material $S = 1$; $\delta, \varepsilon = \mathrm{const}$. From the case $\rho_a = \mathrm{const}$ one can obtain

$$\mathrm{div}\mathbf{q} + \partial\theta/\partial t = -\frac{(\delta-1)}{\rho_a V}\frac{\partial M_s}{\partial t}. \quad (10)$$

Consider the one-dimensional vertical deformation occurring in the deep beds under the influence of a load σ_{zz} of very large horizontal extent. The most simple stress-strain relation is Hook's law for the case of linear isotropic elasticity for one-dimensional problem. In this case the volume strain θ equals the vertical strain. The stress-strain relation is formulated from Eq. (10) as

3. Mechanics of swelling porous media

From (10), with $\rho_a = \rho,\ \delta = 1$, one obtains for case $M_s = \text{const}$

$$\partial\theta / \partial t = \text{div}(D \cdot \nabla\theta),\ D = D(\theta) \tag{11}$$

where $kL / \eta = D,\ L = K + 4G/3,\ \eta$ is the fluid viscosity, k is the permeability. Usually the permeability is the function of volume change so $D = D(\theta)$. Such view of storage equation for swelling soil was obtained and investigated in [3].

4. Mechanics of porous media with solid phase mass changes

In total case the source function $\xi = -\dfrac{(\delta - 1)}{\rho_a V}\dfrac{\partial M_s}{\partial t}$ is not equal zero. It is corresponded to a lot of processes of metamorphism [4]. The most simple relation for ξ is the linear function $\xi = \lambda(\theta_\infty - \theta)^\omega;\ \lambda, \omega, \theta_\infty = \text{const}$. For this case Eq. (10) is transformed in so-called Fisher equation [13]. The theory of solution of this equation gives the expression for the velocity of rising of beds of sedimentary rocks V_r

$$V_r = 2\sqrt{\lambda D} \tag{12}$$

5. Full formulation of the problem

Full formulation of the problem including rheological relations for solid skeleton appears as follows

$$\text{div}\mathbf{q} + \partial\theta / \partial t = \lambda(\theta_\infty - \theta)^\omega \tag{13}$$

$$\mathbf{q} = -\frac{k}{\mu}\nabla p, \tag{14}$$

$$k = k_0 \exp(\alpha\theta),\ \alpha = \text{const} \tag{15}$$

Equation of equilibrium for stress-deformed state of the rocks in Cartesian coordinates [14]:

$$\varepsilon_{ij} = (1/2)(u_{i,j} + u_{j,i}),\ i, j = x, y, z; \tag{16}$$

Differential equations of equilibrium have the following form [15]:

$$\nabla \cdot \sigma_{ij} + \partial p / \partial i = 0;\ \ i, j = x, y, z \tag{17}$$

Rheological relations in case of elastic rheology of skeleton [12, 15] can be given as:

$$\sigma_{ij} = -(K - \frac{2}{3}G)\theta\delta_{ij} - 2G\varepsilon_{ij},\ \theta = \sum_i \varepsilon_{ii};\ i, j = x, y, z \tag{18}$$

The summation over repeated indices is performed, K – bulk modulus of elasticity, G – shear modulus.

Boundary conditions

Problem 1.

$$x, y, z = a : u_x, u_y, u_z = 0;\ \partial p / \partial n = 0$$

$$z = 0,\ p = p_{\max};\ z = L : p = p_{\min}$$

Here a – denotes lateral face of the cube, $z = 0$ is upper boundary (roof), $z = L$ is bottom boundary (bottom). $\theta_\infty = 0,01;\ \omega = 1$. Initial shrinkage is 0.

Problem 2.

$$x, y, z = a : u_x, u_y, u_z = 0;\ \partial p / \partial n = 0$$

$$z = 0, \partial p / \partial z = 0;\ z = L : p = p_{\max}$$

Here a – denotes lateral face of the cube, $z = 0$ is upper boundary (roof), $z = L$ is bottom boundary (bottom). There is an area of higher permeability (fracture) in the center of the cube. $\theta_\infty = -0,01;\ \omega = 1$. Initial shrinkage is 0.

6. Numerical scheme and calculations

Finite difference method (FDM) was used for discretization of the system of Eqs. (13)-(18). Regular cubic grid was constructed in the area of the simulation. Linearization of non-linear coefficients was performed to obtain system of linear algebraic equations [16]. Iterative calculations on each time step were conducted to obtain more stable solution.

7. Results and discussion

Solution of the *Problem 1* is presented in *Fig. 3* and describes formation of fluid-saturated layer during metamorphic dehydration. It is illustrated by the area of increased pressure in the center of the cube in *Fig. 3*. Modulus of volume deformations (deformation is negative in roof and bottom part, and positive in central part of volume) in the area of the process were calculated in relation to the problem of formation of oil deposits in clays with peculiarities that are typical to Bazhenov formation for example. *Fig. 4* demonstrates areas of inhomogeneous deformations in volume. There is the area of decompaction in the center of simulated area, and in the roof and bottom areas there are zones of higher compaction. Such a character of zones of compaction/decompaction prevents filtration of fluid from the central area to the periphery, which is proved out by data from [7].

Problem 2 describes intrusion of liquid magma into vertical fracture (which is oriented along vertical axis of symmetry of the volume of simulation). It was shown that creation of geological structures caused by magmatic intrusions is regulated not only by active phase and capacity of magma chamber but also by interaction of magmatic melts with bearing strata [20, 21]. Such an intrusion is accompanied by alteration of rocks and their physical-mechanical properties. It terms of mathematics it means that solution of governing equation has hyperbolic mode [22]. Presence of non-trivial stationary solutions is a peculiarity for this type of equations. *Fig. 5* demonstrates stationary distribution of pressure in the layer. *Fig. 6* describes configuration of deformations. There are two regions of maximal deformations that form the stationary structures in the layer.

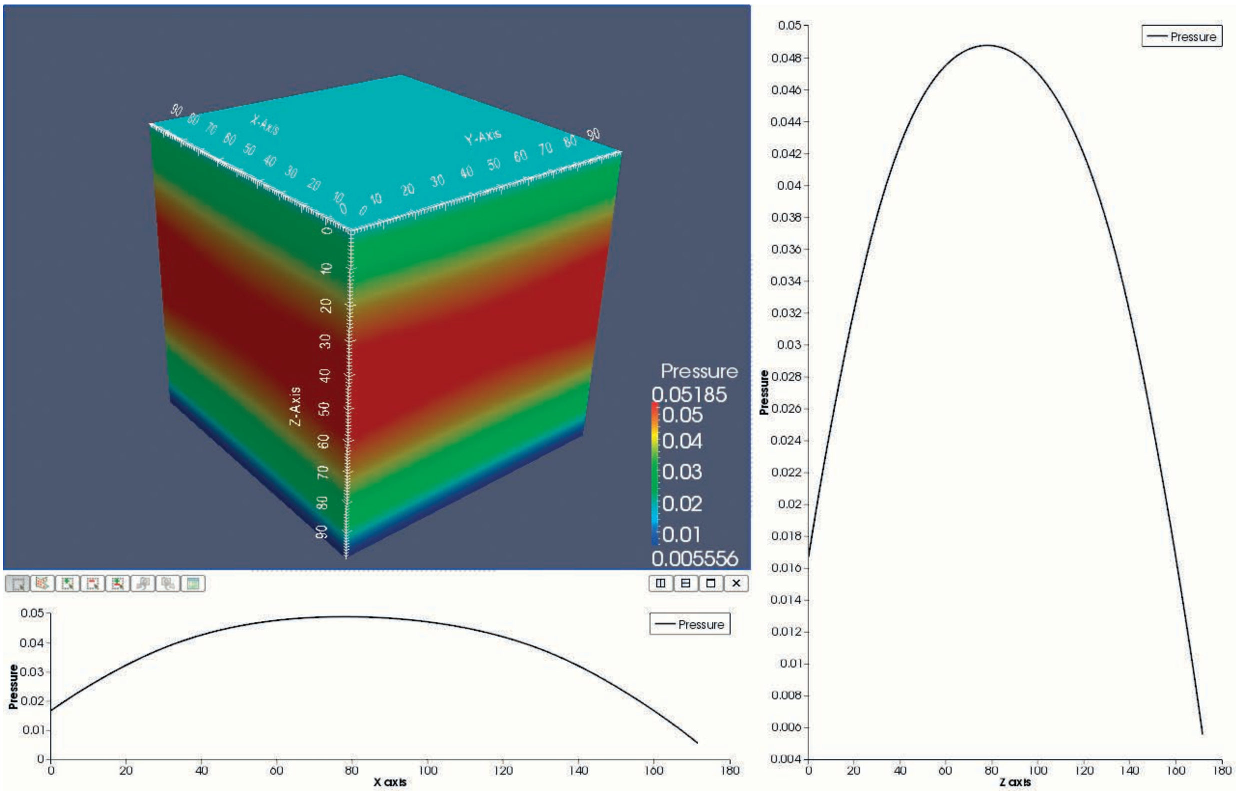

Fig. 3. Formation of fluid-saturated layer during metamorphic dehydration
3. ábra Folyadékkal telített réteg kialakulása metamorfózisos dehidratáció közben

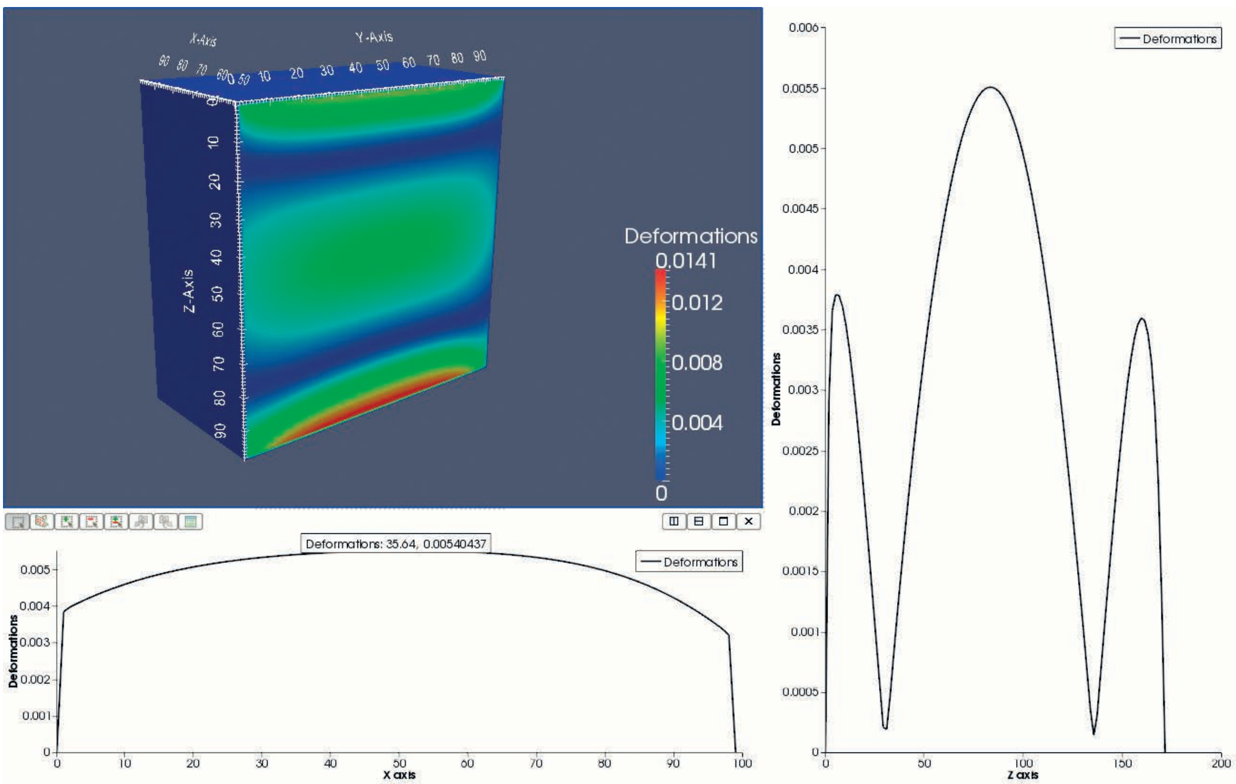

Fig. 4. Areas of inhomogeneous deformations
4. ábra Inhomogén deformáció területei

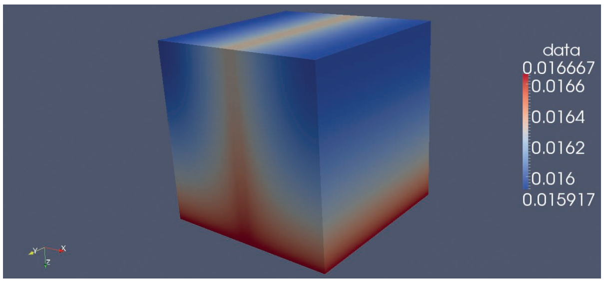

Fig. 5. Stationary distribution of pressure in the layer
5. ábra A réteg nyomáseloszlása állandósult állapotban

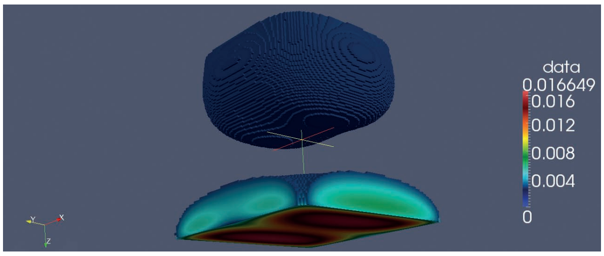

Fig. 6. Configuration of deformations
6. ábra Deformáció elrendeződése

8. Conclusion

Our work belongs to the area of deformation of rocks and metamorphic processes. There are a lot of high quality researches in this area. Influence of stress and deformations on metamorphic processes is examined in [4], non-linear character of swelling is described in [4]. Peculiarities of formation of oil and gas deposits in low permeable rocks are examined in [15]. It is still hard to obtain full model of complex coupled processes which are described by non-equilibrium thermodynamics and rock mechanics on the basis of these results. For example, approaches of rock mechanics often neglect chemical reactions in a rock and concentrate on problems of filtration consolidation, destruction of rocks, fracking, etc.

Our approach is based on the use of volumetric deformation as an effective parameter to obtain correspondent governing equation. Such an approach does not demand to know exact form of equations of chemical kinetics for reactions in rocks. Finally, only one non-linear equation of diffusion-reaction to describe these processes can be obtained. Investigation of complex endogenous processes affords to verify our approach on a wider variety of chemical reactions. We hope that further investigations will help us to clarify real history of rocks.

9. Acknowledgements

This work was supported by RSCF project No. 15-11-10015. The work is performed under the Russian Government Program of Competitive Growth of Kazan Federal University, subsidy for the performing of state assignment in the area of scientific work.

References

[1] Coussy, O. (2004): Poromechanics. *John Wiley & Sons*, 298 p. http://dx.doi.org/10.1002/0470092718

[2] Fjaer, E. – Holt, R. M. – Hoursrud, P. – Raaen, A. M. – Risnes, R. (2008): Petroleum Related Rock Mechanics. 2nd ed. *Elsevier*, 491 p. http://dx.doi.org/10.1016/S0376-7361(07)53023-2

[3] Jaeger, J. C. – Zimmerman, R. W. (2007): Fundamentals of Rock Mechanics, 4th ed., *Wiley*, 488 p.

[4] Charlez, P. A. (1991): Rock Mechanics. *Éditions Technip*, 661 p.

[5] Taron, J. – Elsworth, D. – Min, K-B. (2009): Numerical simulation of thermal-hydrologic-mechanical-chemical processes in deformable, fractured porous media. *International Journal of Rock Mechanics & Mining Sciences*. Vol. 47, pp. 842-854. http://dx.doi.org/10.1016/j.ijrmms.2009.01.008

[6] Kissin, I. G. (2009): Fluids in Earth crust. Geophysical and tectonic aspects. Moscow, *Science* (in Russian)

[7] Bolshakov, Y. A. (1995): Theory of capillary attraction of oil-and-gas accumulation. Novosibirsk, *Science* (in Russian)

[8] Nye, J. F. (1957): Physical Properties of Crystals. *Oxford Press*, 322 p.

[9] Paterson, M.S. (1973): Nonhydrostatic thermodynamics and its geological applications. *Reviews of Geophysics*, Vol. 11, pp. 355-389. http://dx.doi.org/10.1029/RG011i002p00355

[10] McLellan, A. G. (1980): The Classical Thermodynamics of Deformable Materials. *Cambridge University Press*, 338 p.

[11] Hobbs, B. E. – Ord, A. – Regenauer-Lieb, K. (2011): The thermodynamics of deformed metamorphic rocks: A review. *Journal of Structural Geology*, Vol. 33, pp. 758-818. http://dx.doi.org/10.1016/j.jsg.2011.01.013

[12] Verruijt, A. (1984): The theory of consolidation. In: Fundamentals of Transport Phenomena in Porous Media. Part 2: Deformation of Porous Media. *Martinas Nijhoff Publishers*, pp. 351-368.

[13] Fisher, R. A. (1937): The wave of advance of advantageous genes. *Annals of Eugenics*, Vol. 7, No. 4, pp. 355-369. http://dx.doi.org/10.1111/j.1469-1809.1937.tb02153.x

[14] Love, A. E. H. (1944): A treatise on the mathematical theory of elasticity, 4th edition, *Dover Publications*, 672 p.

[15] Nikolaevskiy, N. V. (1996): Geomechanics and Fluidodynamics With Applications to Reservoir Engineering, *Springer*, 352 p. http://dx.doi.org/10.1007/978-94-015-8709-9

[16] Samarskii, A. A. (1989): The theory of difference schemes, Moscow, *Nauka* (In Russian)

[17] Website: https://github.com/ddemidov/amgcl

[18] Demidov, D. E. – Shevchenko, D. V.: Modification of algebraic multigrid for effective GPGPU-based solution of nonstationary hydrodynamics problems. *Journal of Computational Science,* Vol. 3, No. 6, pp. 460-462. http://dx.doi.org/10.1016/j.jocs.2012.08.008

[19] Ahnert, K. – Demidov, D. – Mulansky, M. (2014): Solving ordinary differential equations on GPUs. In: Numerical Computations with GPUs, *Springer*, pp. 125–157. http://dx.doi.org/10.1007/978-3-319-06548-9_7

[20] Bayly, M. B. (1968): Introduction to Petrology. *Prentice-Hall, Inc.,* 371 p.

[21] Hedenquist, J. W., Lowenstern, J. B. (1994) The role of magmas in the formation of hydrothermal ore deposits. *Nature*, Vol. 370, No 6490, pp. 519-527. http://dx.doi.org/10.1038/370519a0

[22] Ortoleva, P. (1994) Geochemical Self-organization. *Clarendon Press*, 411 p.

Ref.:
Khramchenkov, Maxim – **Khramchenkov**, Eduard: *Rheological aspects of underground fluid dynamics and mass exchange processes* Építőanyag – Journal of Silicate Based and Composite Materials, Vol. 68, No. 2 (2016), 34–38. p.
http://dx.doi.org/10.14382/epitoanyag-jsbcm.2016.6

Felszín alatti folyadékdinamikai és tömegáram-folyamatok reológiai kérdései

A cikk bemutatja különböző kőzetanyagok (elsősorban üledékes kőzetek) esetén a poli-ásványos porózus közegben kialakuló folyadék mozgás részletes leírását. A cikk rámutat, hogy egyes esetekben a tározási egyenlet nemlineáris diffúziós egyenlettel írható le. A duzzadásra hajlamos porózus és duzzadásra nem hajlamos talajok esetén a konszolidációt és a folyadék-szemcse kölcsönhatást egyaránt figyelembe kell venni. A cikk illusztrálja különböző kőzetek reológiai viselkedését.
Kulcsszavak: kőzetmechanika, tömegáram, feszültség-alakváltozás állapot, reológiai korrekciók