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## Modeling of non-equilibrium mass-exchange processes in geo-systems

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### ABSTRACT

This paper presents a new mathematical model of coupled processes of filtration, deformations of porous skeleton and mass transfer between solid and liquid phases in sedimentary and igneous rocks. A numerical solution is obtained and processes which can be described by the model are analyzed. Examples of such processes are: formation of a fluid layer along metamorphism of sedimentary rocks, formation of a structure and filtration characteristics of the Bazhenov Shale, appearance of intrusive igneous body (lopolith).

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### 1. Introduction

Mechanics of porous media is the theoretical basis for development of the mathematical models of filtration in deformable porous media, which are used for practical needs, such as civil engineering, petroleum production, and solution of hydro-geological and hydrological problems.<sup>1–3</sup> However, these classical models cannot be easily applied for example in case of interfacial mass transfer, when exact mechanisms of chemical reactions stay unclear. When respective chemical reactions are well-known, mathematical models and their solutions can be obtained.<sup>4</sup> However, when there is no enough information about reaction kinetics the direct approach is inapplicable.

Metamorphic dehydration of sedimentary rocks is one of the examples of such processes. In certain cases metamorphic dehydration can lead to formation of sub-horizontal fluid bodies in the Earth crust.<sup>5</sup> Direct simulation of the process is impossible, since there is no information about the velocity of the dehydration and about the formation time of the fluid body.

Genesis of oil deposits in low permeability clay layers is another example of interfacial mass exchange processes. Oil appears from kerogen as a result of complex process.<sup>6</sup> This process usually occurs in clay layers (source rocks) which contain dispersion of organic remains of ancient flora and fauna. Hereafter,

oil in the form of drops or in the molecular form emerges because of density difference between oil and underground water. Oil usually flocks in so-called “oil traps”. These traps are dome-shaped regions with low permeability vault. Considerable amount of oil stays in the mother rock. Processes which accompany oil formation have significant influence on the structure and filtrational properties of source rocks. The Bazhenov–Abalak Formation in the West Siberia can serve as an example of the oil deposit which was formed in the clayey sedimentary rocks.<sup>7</sup> Information about variation of structure and filtration characteristics of such rocks can be obtained through mathematical simulation. But development of the mathematical model is difficult because there is no exact information about kinetics of transformation of kerogen into oil in the layer.

Intrusion of magma into rocks is another complex geological mass exchange process. Transformation of enclosing rocks material as well as transformation of components of magma occurs within this process and specific structures of igneous rock are formed. Such processes are also hard to simulate, due to the complex nature of chemical transformations.

There are different approaches to development of models of these processes. Hobbs et al.<sup>8</sup> proposed a model which is based on equilibrium and non-equilibrium thermodynamics. In this model reaction–diffusion system is solved for concentrations of active components. Our approach uses dilation as a main variable of the interfacial mass exchange. This method gives an opportunity to develop mathematical model when rate equation for the chemical reaction of the process is unknown.

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## 2. System of general differential equations

In our model we will consider a rock as a porous medium. Material of the porous skeleton takes part in the mass exchange process with the fluid in the pores of the skeleton. The mass exchange process is accompanied by variation of the stress–strain state of the rock. Only some of the components of the porous skeleton take part in the mass exchange process. We will designate the density of these components as  $\rho_s$  and their volume as  $V_s$ .  $V$  is representative elementary volume. Mass balance equation for the fluid which takes part in the mass exchange

$$\frac{\partial \phi S \rho}{\partial t} + \nabla \cdot (\phi S \rho \mathbf{V}) = -j \quad (1)$$

In (1)  $\phi$  stands for the porosity;  $S$  is the fluid saturation;  $\rho$  is the fluid density;  $\mathbf{V}$  is the absolute velocity of the fluid in pores;  $j$  is the rate of the mass exchange.

Mass balance equation for the solid phase

$$\frac{\partial (1 - \phi) \rho_s^t}{\partial t} + \nabla \cdot ((1 - \phi) \rho_s^t \mathbf{W}) = j \quad (2)$$

In (1)  $\rho_s^t$  is the total density of the solid phase;  $\mathbf{W}$  is the absolute velocity of the solid phase. For the mass of the solid phase  $M_s$  in the volume  $V$  we have

$$\begin{aligned} M_s &= \rho_s V_s + \rho_a [(1 - \phi)V - V_s] \\ \rho_s V_s &= M = \text{const} \end{aligned} \quad (3)$$

In (3)  $\rho_s$  is the density of the components of the solid phase, which does not take part in the mass exchange process;  $\rho_a$  is the density of the components of the solid phase, which takes part in the mass exchange.

The dilation of the porous medium

$$\theta = \frac{(V - V_0)}{V_0} \quad (4)$$

Here  $V_0$  is the initial value of  $V$ .  $\theta$  is usually small, so (4) can be written as

$$V = V_0 e^\theta \quad (5)$$

Eq. (5) allows us to obtain from (3)

$$\begin{aligned} M_s &= M(1 - \epsilon) + \rho_a(1 - \phi)V \\ \epsilon &= \frac{\rho_a}{\rho_s} \end{aligned} \quad (6)$$

After differentiation of (6) with respect to time we obtain

$$\frac{\partial M_s}{\partial t} = -M \frac{\partial \epsilon}{\partial t} + (1 - \phi)V \frac{\partial \rho_a}{\partial t} + (1 - \phi)V \rho_a \frac{\partial \theta}{\partial t} - \rho_a V \frac{\partial \phi}{\partial t} \quad (7)$$

where

$$\frac{\partial V}{\partial t} = \frac{\partial (V_0 \exp \theta)}{\partial t} = V_0 \exp \theta \frac{\partial \theta}{\partial t} = V \frac{\partial \theta}{\partial t}$$

For the total density  $\rho_s^t$  and the mass exchange flow  $j$  we have

$$\begin{aligned} \rho_s^t &= \frac{M_s}{(1 - \phi)V} = \rho_a + \frac{M(1 - \epsilon)}{(1 - \phi)V} \\ j &= \frac{1}{V} \frac{\partial M_s}{\partial t} \end{aligned}$$

Then, from (2) it follows

$$\begin{aligned} \frac{\partial}{\partial t} \left[ (1 - \phi) \rho_a + \frac{M(1 - \epsilon)}{V} \right] + \nabla \cdot \left( \left[ (1 - \phi) \rho_a + \frac{M(1 - \epsilon)}{V} \right] \mathbf{W} \right) \\ = \frac{1}{V} \frac{\partial M_s}{\partial t} \end{aligned} \quad (8)$$

After inserting the Eq. (7) into the right-hand side of (8) with regard to  $\mathbf{W} \cdot \nabla \left[ (1 - \phi) \rho_a + \frac{M(1 - \epsilon)}{V} \right] \rightarrow 0^4$  we obtain

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \mathbf{W} \quad (9)$$

From (1) we can have

$$\phi S \frac{\partial \rho}{\partial t} + S \rho \frac{\partial \phi}{\partial t} + \phi \rho \frac{\partial S}{\partial t} + \nabla \cdot (\phi S \rho (\mathbf{V} \pm \mathbf{W})) = -j \quad (10)$$

Designating the filtration velocity as  $\mathbf{q} = mS(\mathbf{V} - \mathbf{W})$  and assuming that  $\mathbf{q} \cdot \nabla \rho$  and  $\mathbf{W} \cdot \nabla (\phi \rho S)$  are infinitesimal we obtain

$$\frac{\phi S}{\rho} \frac{\partial \rho}{\partial t} + S \frac{\partial \phi}{\partial t} + \phi \frac{\partial S}{\partial t} + \nabla \cdot \mathbf{q} + \phi S \frac{\partial \theta}{\partial t} = -\frac{1}{\rho V} \frac{\partial M_s}{\partial t} \quad (11)$$

For the particular case of the single-phase flow, weakly compressible fluid and weakly compressible skeleton we have:  $S=1$ ;  $\rho=\text{const}$ ;  $\epsilon=\text{const}$ ;  $\rho_a=\text{const}$ . Then taking into account (7) Eq. (11) can be written in the following form:

$$\nabla \cdot \mathbf{q} + \frac{\partial \theta}{\partial t} = -\frac{(\rho_a - \rho)}{\rho \rho_a V} \frac{\partial M_s}{\partial t} \quad (12)$$

## 3. Mechanics of porous media with mass-variable solid phase

The source function  $\xi = [(\rho_a - \rho)/(\rho \rho_a V)] \partial M_s / \partial t$  describes a lot of processes of catagenesis and transformation of rock minerals in case of magmatic intrusion.<sup>8</sup> In that work the source function  $\xi$  was expressed through known relations between rate of a reaction and concentration of active components. In case when rate equation for the chemical reaction is unknown, we need to determine  $\xi$  using different approach. For this purpose we make an assumption that metamorphization of rocks comes to an end when dilation reaches some final value  $\theta_\infty$ .<sup>9</sup> Since dilation values are usually small, we can suppose that the rate of change of  $M_s$  is proportional to the difference  $(\theta_\infty - \theta)$  with a certain coefficient  $\lambda$ . We also assume that reactions of mass exchange have different reaction rate at different moments of time, so certain governing parameter  $\omega$  is needed. Taking this into account we obtain for  $\xi$

$$\xi = \lambda (\theta_\infty - \theta)^\omega \quad (13)$$

In the most simple cases for small values of  $\theta$  the parameter  $\omega=1$ .

Now, we can rewrite (12) as

$$\nabla \cdot \mathbf{q} + \frac{\partial \theta}{\partial t} = \lambda (\theta_\infty - \theta)^\omega \quad (14)$$

The Darcy's law

$$\mathbf{q} = -\frac{k}{\mu} \nabla p \quad (15)$$

$$k = k_0 e^{\alpha \theta} \quad (16)$$

Such form of  $k$  was used according to Nikolayevsky.<sup>10</sup>

Equations for the components of the linear strain tensor<sup>11</sup>

$$\epsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (17)$$

The equilibrium equations<sup>10</sup>

$$\begin{aligned} \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + \frac{\partial p}{\partial x} &= 0 \\ \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + \frac{\partial p}{\partial y} &= 0 \\ \frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\partial p}{\partial z} &= 0 \end{aligned} \quad (18)$$

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