THE FORMATION OF MOISTURE AND TEMPERATURE FIELDS IN THE PROCESS OF HEAT- AND MASS-TRANSFER IN HYDROTHERMAL SOLUTIONS WITH ENCLOSING ROCKS

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We consider the mathematical model of the heat- and mass-transfer process in the "hydrothermal solution—enclosing rocks" system and we present a method for the construction of the mathematical model.

In studying the physicochemical processes involved in the interaction of hydrothermal solutions with enclosing rocks, it becomes necessary to study the spacetime distribution of moisture and temperatures about the migration paths of the solutions.

The dynamics of moisture- and temperature-field formation is the most important factor governing the onset and progress of ore formation, of the changes in the rocks surrounding the ore, and of the primary element scattering halos.

In determining the space-time distribution, we have to solve the system of Fourier-Fick partial differential equations describing the processes of heat- and mass-transfer in various media. For a multistratum medium, in general form these equations are represented by the system

$$\begin{aligned} \kappa_{qi} \rho_i \, \frac{\partial t_i}{\partial \tau} &= \operatorname{div} \left(\lambda_i \operatorname{grad} t_i \right) + \xi_i \, r_i \, \frac{c_{mi}}{c_{qi}} \, \frac{\partial U_i}{\partial \tau} \,, \\ \frac{\partial U_i}{\partial \tau} &= a_{mi} \left(\nabla^2 U_i + \delta_i \nabla^2 t_i \right), \end{aligned} \tag{I}$$

where (i = 1, 2, ..., n).

An additional condition ensuring a uniquely defined solution is the behavior of t_i and U_i at the boundaries of the region under consideration.

Since such systems are used to describe a broad class of physical phenomena, it became necessary to develop reliable methods for the solution of the differential equations.

Over several tens of years, such methods have been developed, and they are being used successfully in various branches of science and engineering [1, 2, 4, 7, 8, 10].

However, once we have found the analytical solution for the problems formulated with system (I), we occasionally encounter insurmountable difficulties. These are caused, first of all, by the absence of a universal solution for the system of partial differential equations (I), particularly in the case of combined boundary conditions; secondly, they are a result of the cumbersome nature of the final result which occasionally does not lend itself to physical interpretation.

Therefore, to find a solution for system (I), in studying the process of heat- and mass-transfer for the case of interaction between the hydrothermal solution and enclosing rocks, it is apparently best to use electronic digital-computer procedures to achieve a numerical solution. These methods are based on reduction of the systems of partial differential equations to systems of algebraic equations [1,2,10], or to ordinary differential equations for whose solution we have available standard programs which make use of the approximate methods.

In connection with the fact that our problem is nonlinear and, consequently, cannot be reduced to a system of linear algebraic equations, we set ourselves the goal of compiling a program for the numerical solution of system (I). This problem is considerably facilitated by certain specific features in the geologic objects being studied:

1. The uniformity of heat and moisture distribution as a result of pronounced compression of the tectonic structures which serve as conductors of the hydrothermal solutions (the channels extend for hundreds and thousands of meters and range in width from a fraction of a meter to several meters). The thermal gradient and the moisture-content gradient in the rocks is directed in this case along the normal to the walls of the crack channels.

2. The deep conditions of elevated pressures (to thousands of atmospheres) and elevated temperatures (to $500-600^{\circ}$ C) determine the homogeneous or liquid state of the hydrothermal solutions in which there is virtually no vapor-gas phase. Here we can neglect the (ξ_i) by means of which we account for the heat of liquid-vapor phase transition (I).

With consideration of the above-cited features, we can simplify the system of differential equations (I) to assume the form

$$\begin{aligned} \frac{\partial t_1}{\partial \tau} &= a_{q1} \frac{\partial^2 t_1}{\partial x^2} , \\ \frac{\partial U_1}{\partial \tau} &= a_{m1} \left(\frac{\partial^2 U_1}{\partial x^2} + \delta_1 \frac{\partial^2 t_1}{\partial x^2} \right) , \\ \frac{\partial t_2}{\partial \tau} &= a_{q2} \frac{\partial^2 t_2}{\partial x^2} , \\ \frac{\partial U_2}{\partial \tau} &= a_{m2} \left(\frac{\partial^2 U_2}{\partial x^2} + \delta_2 \frac{\partial^2 t_2}{\partial x^2} \right) , \end{aligned}$$
(II)

The boundary conditions for the uniquely defined solution of this system are the following:



Fig. 4. Change of temperature (a) and moisture content (b) in granites ($\lambda_q = 3.0 \text{ kcal/m} \cdot \text{hr} \cdot \text{deg}$, $a_m = 0.00005 \text{ m}^2/\text{hr}$): 1) $\tau = 5 \text{ hr}$; 2) 15; 3) 20; 4) 30; 5) 50; 6) 75.

the thermal conductivities (λ_q) (Figs. 1-4). Indeed, if a clayey shale is heated to a temperature of t = 40° C at a distance of 2 m from the channel within a period of time τ = 700 hr (Fig. 3), a diatomite slab will be heated within a period of time τ = 500 hr. For granites exhibiting a relatively high thermal conductivity, the heating to a temperature of 40° C at this distance will be completed within only 65 hr (Fig. 4). The moisture field, in turn, also exerts significant influence on the temperature distribution in the "hydrothermal solutionenclosing rocks" system.

For example, the heating rate for "dry" granites (in calculating the temperature distribution we assumed that they were impermeable to moisture [6]) lags considerably behind the rate of heating granite exhibiting the same thermal conductivity, but where consideration is given to the diffusion of the solution from the crack channel into these granites (Fig. 4).

Here we have not yet taken into consideration the change in the thermal conductivity whose magnitude increases sharply as the moisture content of the rocks is increased [5,7,9,11].

Consequently, having determined the temperature within and around any channel filled with the thermal solution, we must account not only for the relationship of the thermal conductivity to temperature and moisture (i.e., the effective thermal conductivity $\lambda_{eff} = f(t, U)$), but also to the moisture gradient in the rocks.

An interesting phenomenon is the appearance of "temperature stagnation zones" in the heated rocks and their presence for a prolonged period of time. Such zones are formed where the isochrones intersect at the nodes whose coordinates are strictly fixed for the corresponding rocks (Figs. 1-4). The physical interpretation of the factors responsible for such an effect can be determined through special studies.

NOTATION

x is the instantaneous coordinate, m; τ is the time coordinate, hr; t is the temperature, °C; U is the moisture content, kg/kg; λ_q is the thermal conductivity, kcal/m · hr · deg; c_q is the heat capacity, kcal/kg · deg; ρ is the density, kg/m; λ_m is the moisture conductivity coefficient, kg/m · hr · °M; *a* is the thermal diffusivity (*a*_q), and moisture diffusivity (*a*_m), m²/hr; δ is the thermal gradient, kg/kg · deg; r is the specific heat of evaporation, kcal/kg; ξ is the evaporation criterion ($0 \le \xi \le 1$); $\nabla =$ grad = $(\partial/\partial x + \partial/\partial y + \partial/\partial z)$ is the gradient; $\nabla^2 = (\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2)$ is the Laplace operator; h is the grid pitch.

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14 November 1967 Ins

Institute of Geochemistry Siberian Division AS USSR, Irkutsk the initial conditions

$$t(\mathbf{x}, \tau) \mid_{\tau = 0} = \begin{cases} t_0 \text{ when } 0 < x < l, \\ t'_2 \text{ when } l < x < \infty, \end{cases}$$
(1)

$$U(x, \tau)|_{\tau=0} = \begin{cases} U_0 = \text{const when } 0 < x < l, \\ U'_2 & \text{when } l < x < \infty, \end{cases}$$
(2)

the boundary conditions

$$\lambda_{q1} \left. \frac{\partial t_1(x, \tau)}{\partial x} \right|_{x=l} = \lambda_{q2} \left. \frac{\partial t_2(x, \tau)}{\partial x} \right|_{x=l} , \qquad (3)$$

$$\lambda_{m1} \frac{\partial U_1(x,\tau)}{\partial x}\Big|_{x=l} = \lambda_{m2} \frac{\partial U_2(x,\tau)}{\partial x}\Big|_{x=l}, \quad (4)$$

$$\frac{\partial t_1(x,\tau)}{\partial x}\Big|_{x=0} = 0, \tag{5}$$

$$\frac{\partial U_1(x,\tau)}{\partial x} = 0, \qquad (6)$$

$$t_{2}(x, \tau)|_{x \to \infty} = t'_{2} = \text{const},$$
(7)
$$U_{2}(x, \tau)|_{x \to \infty} = U'_{2} = \text{const}.$$
(8)

Thus the system of equations (II) is a mathematical model of a two-stratum medium consisting of a singlephase liquid hydrothermal solution ($0 \le x \le l$) including enclosing rocks of various porosities ($l \le x < \infty$) and a boundary of separation (l).

Here we examine half the axisymmetric channel (boundary condition (5)).

We assume that the solution $(t = 350^{\circ} \text{ C})$ instantaneously fills the crack channel and cools therein, interacting with the side rocks (initial conditions (1) and (2)). Here the mass of the solution is considerably greater than that of its fraction which diffuses into the rocks, since the over-all volume of the pores filled with the solution is incomparably small in comparison with the channel volume. The amount of the solution in the crack channel is therefore assumed to be constant (initial conditions (2) and (6)).

For the derived system (II), with consideration of the initial and boundary conditions, we compiled a program for its solution on a BESM-2M computer. The program is based on a method of finite differences (or grids) which is used for a broad class of equations in mathematical physics [1,2,10]. The essence of this method lies in the fact that the domain($(D = \{0 \le x < < \infty\})$ of continuous change in the argument (in our case, the space coordinates x) is replaced by a discrete set of points ($D_h = \{x_i = ih, 0 \le x \le l; x_i = l + ih, l < x < < \infty$) in geometric space (x_i). Then, instead of the continuous-argument function we obtain the discrete-argument function ($f(x, \tau) \approx f_i \times (ih, \tau)$). We choose a set of points (x_i) so as to satisfy boundary conditions (7) and (8) at the point (P).

The derivatives with respect to x in the equations of system (II) are approximately by the difference ratios

$$\frac{\partial f(x,\tau)}{\partial x} = \frac{f(x+h,\tau) - f(x-h,\tau)}{2h} + R_1(h),$$
$$\frac{\partial^2 f(x,\tau)}{\partial x^2}$$
$$- \frac{f(x+h,\tau) - 2f(x,\tau) + f(x-h,\tau)}{h^2} + R_2(h),$$

where

1

$$R_{I}(h) \leqslant \frac{h^{2}}{3!} \max_{x-h \leqslant x \leqslant x+h} f^{III}(x, \tau)$$

and

$$|R_2(h)| \leq \frac{2h^2}{4!} \max_{x-h \leq x \leq x+h} f^{\text{IV}}(x, \tau)$$

are errors in the approximation of the derivatives.

As a result of all these transformations, the system of partial differential equations (II) with consideration of the corresponding boundary and initial conditions changes into a system of ordinary differential equations, solved for the derivative with respect to time (τ) of the sought functions:

$$\begin{split} \frac{dt_1}{d\tau} &= \frac{9a_{q1}}{l^2} (t_2 - t_1), \\ \frac{dt_2}{d\tau} &= \frac{9a_{q1}}{l^2} (t_1 - 2t_2) + \frac{9a_{q1}}{l^2 \left(\frac{3\lambda_{q1}}{l} + \frac{5\lambda_{q2}}{p - l}\right)} \\ &\times \left(\frac{3\lambda_{q1}}{l} t_2 + \frac{5\lambda_{q2}}{p - l} t_3\right), \\ &\frac{dt_3}{d\tau} &= \frac{25a_{q2}}{(p - l)^2} (t_4 - 2t_3) \\ &+ \frac{25a_{q2}}{(p - l)^2 \left(\frac{3\lambda_{q1}}{l} + \frac{5\lambda_{q2}}{p - l}\right)} \\ &\times \left(\frac{3\lambda_{q1}}{l} t_2 + \frac{5\lambda_{q2}}{p - l} t_3\right), \\ &\frac{dt_4}{d\tau} &= \frac{25a_{q2}}{(p - l)^2} (t_5 - 2t_4 + t_3), \\ &\frac{dt_6}{d\tau} &= \frac{25a_{q2}}{(p - l)^2} (t_6 - 2t_5 + t_4), \\ &\frac{dt_6}{d\tau} &= \frac{25a_{q2}}{(p - l)^2} (t_5 - t_p), \\ &\frac{dU_3}{d\tau} \\ &- \frac{25a_{m2}}{(p - l)^2} \left(U_4 - 2U_3 + U_9\right) + \frac{25a_{m2}\delta}{(p - l)^2} (t_4 - 2t_3) \\ &+ \frac{25a_{m2}\delta}{(p - l)^2} (U_5 - 2t_4 + t_3), \\ &\frac{dU_4}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2U_4 + U_3) \\ &+ \frac{25a_{m2}\delta}{(p - l)^2} (t_5 - 2t_4 + t_3), \\ &\frac{dU_4}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2U_4 + U_3) \\ &+ \frac{25a_{m2}\delta}{(p - l)^2} (t_5 - 2t_4 + t_3), \\ &\frac{dU_5}{(p - l)^2} \left(\frac{3\lambda_{q1}}{t} + \frac{5\lambda_{q2}}{p - l} (U_5 - 2U_5 + U_4) \\ &+ \frac{25a_{m2}\delta}{(p - l)^2} (t_6 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2U_5 + U_4) \\ &+ \frac{25a_{m2}\delta}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)^2} (U_5 - 2t_5 + t_4), \\ &\frac{dU_6}{d\tau} &= \frac{25a_{m2}}{(p - l)$$

For the derived system (III) we compiled a program for its solution on a BESM-2M computer (with introduction of the additional equation $d\tau/d\tau = 1$), which involves calculation of the right-hand members of the equations and the processing of these results.

Provision is made in the proposed program for switching to the standard program (compiled by the Computer Center of the USSR Academy of Sciences), which makes use of the Adams method and provides for automatic selection of the time step.

The resulting solution of $t_i(x, \tau)$ and $U_i(x, \tau)$ (Figs. 1-4) differs from the sought solution by no more than

0.03
$$\max_{\xi \in \mathbf{X}} f^{\mathrm{IV}}(\xi, \tau)$$

In this formulation of the problem, such an error is quite acceptable. The program for the numerical solution of systems such as the one under consideration permits us to find the distribution of the temperatures and moisture contents for the most varied of rocks, soils, and construction materials, in which the physical properties vary over a wide range.

We investigated the process of heat- and mass-transfer in the formation of the moisture- and temperaturefields for sandstones, clayey shales, granites, and diatomite slabs (Figs. 1-4). The data on their thermophysical properties and the properties of moisture conduction were taken from the various papers by A. V. Luikov [7,8], E. A. Lyubimova, G. N. Starikova, and A. P. Shushpanov [9], V. N. Kobranova [5], and A. F. Chudnovskii [11].

A common and characteristic feature of most rocks is the relatively rapid rate of heating in comparison with the rate at which they take up moisture from the hydrothermal solution. An apparent exception is represented by the large-grain rocks, since even in the case of small-grain sandstones we find no marked difference between the transport of energy and matter (Fig. 1).



Fig. 1. Change of temperature (a) and moisture content (b) in $(\lambda_q = 1.1 \text{ kcal/m} \times \text{hr} \cdot \text{deg}, a_m =$ = 0.0012 m²/hr: 1) $\tau = 3 \text{ hr}$; 2) 50; 3) 100; 4) 200; 5) 400.



Fig. 2. Change of temperature (a) and moisture content (b) in diatomite slab ($\lambda_q = 0.2 \text{ kcal/m} \cdot$ $\cdot \text{hr} \cdot \text{deg}, a_m = 0.00005 \text{ m}^2/\text{hr}$): 1) $\tau = 3 \text{ hr}$; 2) 30; 3) 50; 4) 100; 5) 200; 6) 300; 7) 400; 8) 500; 9) 600.

The greater the porosity of the rock, the more clearly defined the delay in the propagation of the moisture front relative to the motion of the heating front (Figs. 2-4). Consequently, the diffusion of the solution in rocks is a function of their porosity and the associated coefficient of moisture transport (a_m) . However, this is not a uniquely defined relationship, since the moisture field is formed in previously heated rocks in which the effect of the thermal-gradient coefficient $[\delta]$ is evident, i.e., $U = f(a_m, \delta)$.

On the other hand, the distribution of temperatures in rocks of any porosity is determined primarily by



Fig. 3. Change of temperature (a) and moisture content (b) in clayey shales ($\lambda_q = 0.3 \text{ kcal/m} \cdot \text{hr} \cdot \text{deg}$, $a_m = 0.0004 \text{ m}^2/\text{hr}$: 1) $\tau = 15 \text{ hr}$; 2) 50; 3) 100; 4) 200; 5) 300; 6) 400; 7) 500; 8) 700.