RESEARCH ON HEAT AND MASS TRANSFER IN GEOLOGICAL HETEROGENEOUS SYSTEMS (SURVEY)

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Inzhenerno-Fizicheskii Zhurnal, Vol. 13, No. 6, pp. 945–954, 1967

UDC 536.241

Many geologists now employ the methods of mathematical physics to study the physicochemical processes that take place in the earth's crust: geothermal and hydrothermal processes of mineral and ore formation, crystallization of magmatic melts and hydrothermal solutions, recrystallization of country rock, etc.

Since one of the principal factors governing these processes is temperature, considerable research has naturally been done in that direction.

The first attempts to construct mathematical models of the temperature fields relating to certain geological processes were made at the beginning of this century. Particularly intense research began in the 'thirties. Thus, Jones [43] examined the relationship between temperature fields and ore bodies, Schneiderhohn [52] attempted to establish the relation between the formation of various mineral associations and the temperature-time cooling curves of the intrusions. However, these were still rather narrow and specialized problems.

Lovering's work [20, 48–50] was more extensive. He worked out the mathematical basis of heat transfer in its relation to geological problems [20], and, using Ehrenburg's equation [38], calculated the temperature-time curves at the contact of different kinds of rocks [48]. In [49], reviewing the literature up to 1952, Lovering deals with the various methods of measuring and calculating temperatures.

Lovering has paid special attention to the problem of the time of formation of an intrusion. He considers that "when the time of formation of an intrusion is short as compared with the cooling time, the mathematical assumption (concerning the temperature field associated with the one-shot injection of magma—author's note) is completely justified." The multiple injection of a magmatic melt results in a considerable change in cooling time and the temperature distribution is almost impossible to determine.

Lovering emphasizes the significance of the latent heat of crystallization, which has an important influence on the conservation of temperature by the walls surrounding the moving magma. Since in these circumstances insuperable mathematical difficulties are often encountered, he has found it possible to use the method of thermal models, the most reliable for an objective evaluation. Lovering also stressed the importance of taking into account the latent heat of fusion during the crystallization of magmatic melts in his subsequent publications [20]. He established that for melts with different crystallization intervals the solidification times (τ_1 and τ_2) "vary as the square of the ratio of the parameters λ during the early stages of crystallization," i.e.,

$$\tau_1 = \tau_2 \left(\frac{\lambda_1}{\lambda_2}\right)^2,$$

where λ is the root of the equation

$$\frac{1-\operatorname{erf}(b\lambda)}{1+\operatorname{erf}(\lambda)} \exp\left[(b^2-1)\lambda^2\right] = a\,\frac{T_1 - T_0}{T_1}.$$

The same subject was examined by Larsen in [46], where he calculated the temperature fields and cooling time of batholiths and presented the cooling curves and temperature gradient in the batholith and the lateral rocks. Larsen assumed the absence of a geothermal gradient, which considerably reduces the value of his calculations. He also attempted to take into account and estimate the latent heat of fusion in terms of an additional specific heat of fusion, by introducing the rate of displacement of the crystallization front. For this purpose he employed the mathematical equation (equation for the case of thin ice)

$$\frac{dx}{d\tau} = \frac{kT_{\text{cryst}}}{\rho x}.$$

But this assumption is too remote from actual geological processes.

During those years Ingersoll, Zobel, and Ingersoll [39] published a monograph that became a sort of manual of the general theory of heat conduction in relation to geology. By means of a permissible simplification of the thermal process, it became possible to describe it mathematically. However, it was necessary to find simple solutions of the differential Fourier equation (intelligible to geologists) for the final computations. These solutions and the mathematical approach to them are also given by the authors for certain geological situations, such as heat transfer between a spherical body, a flat slab, or a parallelepiped and a cold surrounding medium.

The same authors examined the problem of the duration of cooling of such bodies and derived a time rule: the time required to reach identical temperatures at two points in space is directly proportional to the square of the distance between them, i.e., $\tau \backsim r^2$. A corollary of this rule is their conclusion concerning the similarity of time and the possibility of simulating it in geological processes.

Somewhat later, Kazanli [11–14] became preoccupied with calculating the temperature fields of an intrusion. He demonstrated the effect of the temperature factor on the zonality of hypogenetic mineralization and its role in ore formation. "In the formation of metal-bearing veins and skarn zones the principal role was played by the thermal effect due to the heat of the intrusion.... And the temperature field of the apical parts determined the zonal arrangement of the ore deposits."

Kazanli constructed the following mathematical model of the temperature field for a spherical body:

$$T=\frac{T_0}{2}\left[\operatorname{erf}\left(\frac{R-x}{2\sqrt{a\tau}}\right)+\operatorname{erf}\left(\frac{R+x}{2\sqrt{a\tau}}\right)\right]+$$
$$+\frac{T_0\sqrt{a\tau}}{x\sqrt{\pi}}\left[\exp\left(-\frac{R+x}{2\sqrt{a\tau}}\right)^2-\exp\left(-\frac{R-x}{2\sqrt{a\tau}}\right)^2\right].$$

Using the temperature distribution obtained, he attempted to establish the temperature intervals of crystallization of various minerals and calculate the intrusion formation time.

The relationship between mineralization zones and temperature fields was analyzed by Kropotkin [19] and Shcuv [51].

The work of Jaeger [40–42] is distinguished by thorough research and by exact mathematical calculations and their geological interpretation. Like previous investigators, he assumes that the zones of ore deposits depend on the temperature field and shows that the calculations are affected by taking into account, even in the first approximation, phase transitions during the crystallization of the magma [40]:

$$T_{\text{cryst}}=\frac{T_1}{1+\operatorname{erf}(C)}\left(1+\operatorname{erf}\left(\frac{R}{2\sqrt{a_1\tau}}\right)\right),$$

where C is the root of the equation

$$\frac{1+\operatorname{erf}(bC)}{1+\operatorname{erf}(C)}\exp[(b^2-1)C^2]=a\frac{T_1-T_0}{T_1}.$$

Jaeger [37, 41] also takes into account the latent heat of fusion L_1 in calculating the temperature T_c of the magma at the contact with the surrounding rock:

$$T_c=\frac{sT_1}{s+\operatorname{erf}(\lambda_1)},$$

where λ_1 is the root of the equation

$$\lambda_1(s+\operatorname{erf}(\lambda_1))\exp(\lambda_1^2)=C_1T_1/L_1\pi^{1/2}.$$

Jaeger proposes a method of calculation for the case of magma intrusion into wet country rock with allowance for the latent heats of crystallization and evaporation. In this system the magma solidification time can be obtained from the formula

$$\tau_s=\frac{2D^2}{\lambda_1^2\alpha_1}10^{-5}\text{ (yr)}.$$

Jaeger performed a great service in first drawing attention to the possibility of mass transfer in rocks under the influence of the temperature gradient of a magmatic melt. True, he did this indirectly by introducing the latent heat of evaporation into the equation. As a result he derived a formula for the vapor front (plane of width D_s):

$$D_s=D\frac{\lambda_0\alpha_0^{1/2}}{2\lambda_1\alpha_1^{1/2}}.$$

The temperature distributions in the crystallizing magma and in the wet country rock can be expressed by the terms λ_0 and λ_1, which are roots of the equations

$$\begin{cases}\lambda_1\exp(\lambda_1^2)[q\operatorname{erf}(\lambda_1)+\operatorname{erf}(r_1\lambda_0)]=\\ \quad=q(T_1-T_0)C_1/L_1\pi^{1/2},\\ [T_0\exp(-b^2\lambda_0^2)+(\lambda_0 pL_0\rho''\pi^{1/2}/\rho_0C_0)]\times\\ \quad\times[q\operatorname{erf}(\lambda_1)+\operatorname{erf}(r_1\lambda_0)]=\\ \quad=s(T_1-T_0)\exp(-r_1^2\lambda_0^2)\operatorname{erfc}(b_1\lambda_0).\end{cases}$$

(The subscript 1 refers to magma, 0 to wet rock, while subscriptless quantities relate to dry rock.)

The ability of magmas to participate in mass transfer and assimilate material from the surrounding medium was later investigated by Kadik and Khitarov [9, 10], who succeeded in obtaining a quantitative estimate of the probability of these assumed interaction processes.

In order to characterize the magma flows they used hydrodynamic models, which enabled them to obtain mass-transfer criteria. On the basis of Lighthill's work [47], it was shown that, in the presence of certain temperature drops, regions of stagnation, which determine the zonality of mineralization, develop. The investigators determined the critical channel radii at which stagnation zones are possible:

$$R_{\min}=\left(4.45\cdot10^9\frac{l}{T_1-T}\right)^{1/4},$$
$$R_{\max}=\left(4.45\cdot10^{15}\frac{l}{T_1-T}\right)^{1/4},$$

where T is the temperature of the melt on the axis at the cold end of the channel.

It was found that the quantity $I=f(\text{const}/\mu)$ can be used to estimate the effect of temperature on the mass-transfer rate in terms of viscosity, i.e., $\mu=F(T)$. Hence it follows that an exceptionally strong influence on mass transfer is exerted by the presence of water in the melt, i.e., it is necessary to establish the laws governing the water balance in the magma and the country rock.

It is interesting to note that Vinogradov [2], Magnitskii [27], and others explain the mass-transfer mechanism in the same way as the process of zone refining. Magnitskii has reached a number of interesting conclusions in relation to the distribution of the principal ore- and rock-forming minerals, which are in good agreement with actual geological observations.

The effect of the heat of crystallization of the cooling magma on the temperature distribution and heat balance in the melt-rock system, also noted by Jaeger [40], is taken into account in the work of Sharapov and Melamed [36]. They investigated the process of formation of dikes, which are formed when "dry" magma is injected into cracks and large cavities in the earth's crust.

When the "dry" magma cools, a crystalline layer that varies with time $x = \xi(\tau)$ is formed at the contact with the cold rock. At this moving boundary of constant temperature (T = const), the heat of phase transition $Q\xi'(\tau)$ of the magma is released.

The authors used the familiar Stefan problem to construct the temperature field of the cooling intrusion. The heat $Q\xi'(\tau)$ was taken into account by the boundary condition of equality of the heat fluxes at the moving interface between the solid and liquid phases:

$$k_2 \frac{\partial T_2}{\partial x}\bigg|_{\xi(\tau)} - k_1 \frac{\partial T_1}{\partial x}\bigg|_{\xi(\tau)} = Q\xi'(\tau),$$

where the subscript 1 denotes the magma, and the subscript 2, the rock. This condition immediately imposes a certain limitation on the applicability of the final conclusions. In fact, this formulation of the problem is legitimate only for rocks whose thermophysical characteristics are the same as or similar to the characteristics of the crystallized magmas.

The authors then point out that their value for the intrusion crystallization time is less than follows from the data of Jaeger and Carslaw [37, 40]. Here it should be noted that Jaeger did not take into account the displacement ($x = \xi(\tau)$) of the magma crystallization front, whereas Sharapov and Melamed did, though they did not show how it was determined. This possibly subjective approach may have led to a certain error in their calculations. Moreover, the numerical solution of the problem on an IG-1 integrator also introduces a certain error, to which we have alluded in [17, 31]. The work of Sharapov and Melamed is specially valuable in that they demonstrated the dynamics of the temperature field in the presence of a moving magma crystallization front.

It is characteristic that all the publications cited above are concerned with magmatic melts and not with thermal solutions. The reason for this is simple: magmatic melts, having a high viscosity and density, cannot diffuse into the surrounding rock (the diffusion of gases and vapors is disregarded), and thermal interaction is based exclusively on heat conduction.

In the case of hydrothermal processes, however, where moving aqueous solutions are involved, it is impossible to avoid taking into account mass exchange with the surrounding rock, and this introduces certain difficulties into the mathematical description of the process. Accordingly, research in this area is, as it were, heading in two directions at the same time—the study of pure heat transfer and the study of mass transfer between the thermal solutions and the rock.

Laffitte's work [44, 45] is not free from this shortcoming. He examines the temperature distribution around a hydrothermal channel using the known function

$$T = T_0 \operatorname{erf}\left(\frac{x}{2\sqrt{a\tau}}\right).$$

To maintain a constant temperature in the channel walls, the flow Φ of solution must vary according to the law

$$\Phi = \frac{2kT_0}{c\nu\sqrt{\pi a\tau}}.$$

Consequently, to maintain a constant temperature, the flow of solution must decrease with time.

In this case, then, the formation of a vein is due not to a fall in the temperature of the solution, since it will vary only slightly, but to a change in pressure, and, hence, a decrease in the solubility of the water.

Laffitte has indicated the possibility of determining the time of formation of a body and constructed time-temperature cooling curves for a thermal solution. For this model of the thermal process, the heating front in the surrounding rock must remain constant and must correspond to a zone of metamorphism of perfectly definite dimensions.

In [17, 31] we investigated certain models of the temperature fields in the "hydrothermal solution–country rock" system. In this case we also assumed the absence of mass transfer, which introduced a certain error into our conclusions concerning the temperature distribution and cooling time.

Ogilvy [29, 30] examines geotemperature fields from a somewhat different standpoint. He gives a method of calculating them in relation to subsurface water surveys. Ogilvy also assumes that in the depths of the earth's crust the law of molecular heat conduction, i.e., Fourier's law, basically applies. He takes mass transfer into account, not that associated with the interaction of thermal springs and the country rock, but the natural, usually vertical percolation of subsurface water (at the rate ω) closer to the surface. Then the temperature waves have the form

$$T - \bar{T} = A_0 \exp\left[-\left(\frac{w}{2a} + \gamma\cos\varphi\right)x\right] \times$$
$$\times \cos\left(\frac{2\pi\tau}{t} - \gamma x \sin\varphi\right).$$

Both theory and practice indicate that, for sufficiently weak subsurface-water percolation, the geothermal field is distorted.

In the first approximation it may be assumed that the heat flux

$$\bar{q} = \omega\rho H + k\frac{\partial T}{\partial x}.$$

In the steady state, which is actually observed,

$$T - T_0 = \frac{g_0}{p}[1 - \exp(-px)].$$

Ogilvy offers a temperature wave equation for an inhomogeneous medium and notes the possibility of an approximate evaluation of the time during which temperature anomalies—relic temperatures—persist.

Later [30], he considered the effect of surface temperature T_{h0} on the temperature field of the neutral layer (surface separating the upper zone h_0 in which the heat flow is subject to the annual temperature fluctuations of the earth's surface). He assumes that, in the first approximation it is possible to use an exponential dependence of the attenuation of the temperature oscillations with depth: $h > h_0$. Then

$$T(h) = \overline{T}_{h_0} + \frac{I_s}{k}(h - h_0) + $$
$$+ A_{h_0} \exp\left[-\sqrt{\frac{\pi}{\alpha t}}(h - h_0)\right] \times$$
$$\times \cos\left[\frac{2\pi\tau}{t} - \sqrt{\frac{\pi}{\alpha t}}(h - h_0)\right].$$

White [53–55] has also investigated the behavior of the temperature gradient in regions of intense hydrothermal activity, noting that near the surface this gradient is very high (23° at 30 m). He relates hydrothermal ore deposits to such regions.

The presence and character of hydrothermal changes in the wall rocks and data on modern thermal springs and geysers enabled White to estimate the duration of these processes.

A comprehensive investigation of the hydrothermal characteristics of the volcanic region of Kamchatka has been made by a group of workers from the Institute of Vulcanology of the Siberian Division AS USSR: B. G. Polyak, E. A. Vakin and E. N. Ovchinnikova [33]. In addition to the conditions of thermal spring formation, the water-bearing properties of the rocks, and the nature of the fracture zones, they studied the effect of a magmatic center on the regional geotemperature field. Polyak and his colleagues give a mathematical model for the corresponding boundary conditions and construct the isotherms around the magnetic chamber—the focus of the thermal springs.

The investigators did not take into account the effect of subsurface water convection and the geothermal gradient, which, of course, introduced a corresponding error into their final results.

The effect of the temperature distribution in the rock and the time factor on the formation of hydrothermal deposits was investigated by Rundkvist [34, 35].

Problems connected with the study and utilization of hot springs were examined at conferences in 1961 and 1966 [3, 32]. At these conferences a number of interesting papers were read: Nazarov [28] reported on the utilization of the earth's heat; Krasintseva and Shcherbakov [18] suggested the tempting idea of creating artificial geothermal deposits; and Makarenko [26] presented his study of the effect of subsurface waters on the distribution and dissipation of plutonic heat. On the basis of his own observations, the latter drew a number of interesting conclusions.

In the interior of the earth under the action of heat, even at low temperatures (100° C), the bound water of the rocks goes over into the free state and becomes very mobile, thus increasing the permeability of the rocks.

In the presence of adiabatic absorption of heat by the solution, large negative anomalies develop. Accordingly, the internal water, moving through the rock, displaces and regionally deforms the temperature fields and, apparently, in places "cuts off" the heat flow. The analytical calculation and simulation of the thermal fields depend upon the availability of information about the thermophysical characteristics of the geological objects of investigation. Only if they are known can geologists use models for practical calculations. At present, reliable data on thermophysical characteristics can be obtained only as a result of experimental research. Accordingly, there has been much activity in this direction. Particularly useful work has been done by Kobranova [15] and Lyubimova, Starikova, and Shushpanov [25] in connection with the physical properties of rocks. The same problems have engaged the attention of Korotnikova [16], who has investigated the relation between internal heat and the thermal coefficients of rocks. Zharkov [4] has studied the thermal conductivity of the earth's crust, Aerov and Umnik [1] the thermal conductivity in a granular bed, and so on.

We have already noted that in the area of geothermal processes there have been few studies of heat and mass transfer; on the other hand, considerable progress has been made in this respect in connection with the cryolithic zone.

A comprehensive investigation of heat and mass transfer in frozen soils is being successfully conducted at the Institute of Geocryology of the Siberian Division AS USSR under the direction of N. S. Ivanov [5–8].

The apparatus of mathematics and simulation are widely used in studying these processes. A number of mathematical models have been constructed, and a large number of final calculations, completely explaining the processes of heat and mass transfer in frozen soils, have been made. Workers at the Institute have developed various pieces of experimental apparatus for investigating the moisture and temperature fields and for determining the thermophysical characteristics of rocks.

The research of N. S. Ivanov convincingly demonstrates not only the need, but also the possibility, of solving the problem of heat and mass transfer in connection with hydrothermal processes of mineral and ore formation. The work of Luikov and Mikhailov [21–24] who have formulated the mathematical problem and provided methods of solving it, may prove invaluable in relation to the study of heat and mass transfer in geological systems. By analyzing their models of the moisture and temperature fields, it is possible to obtain a correct understanding of the mechanism of interaction of thermal solutions and the wall rock, and to predict the probability of certain chemical reactions both in the solution itself and in the rock.

From this standpoint, it is possible to arrive at a quantitative interpretation of such processes, and estimate the time of formation of hydrothermal bodies.

Thus, in the area of formation of intrusive bodies, the mechanism of thermal interaction between the magma and the surrounding rock has been quite thoroughly studied. Reliable methods of describing the resulting temperature fields in mathematical terms have been found, and the possibility of determining the intrusion cooling time has been demonstrated. An attempt has been made to establish a relationship between the zonality of the transformations in the neighborhood of the ore and the temperature distribution in the wall rock.

In constructing models of the temperature fields associated with hydrothermal processes the investigators have failed to take into account the effect of mass transfer between the thermal solution and the rock, which considerably reduces the value of the results obtained. It is necessary to study the mechanism of heat and mass transfer in "thermal solution-country rock" systems by the methods of mathematical and physical modeling (i.e., experiment) of natural hydrothermal processes.

The lack of reliable information about the thermophysical characteristics of thermal solutions and country rocks considerably reduces the practical value of analytical studies.

The determination of these thermophysical characteristics, true and effective, is an urgent problem for geologists, since it would make it possible to turn the analytical models into an effective apparatus for practical calculations.

NOTATION

x, y, and z are coordinates; τ is the crystallization time of the solutions and melts, hr; R is the thickness of the channel, m; l is the height of the channel, m; r is the distance between two points in space, m; D is the width of the solidification band, m; T is the temperature (° C) varying in space and time; T_0 is the initial temperature (°C) of solutions and melts; T_{cryst} is the temperature (°C) of crystallization of the solutions and melts; $\bar{T}$ is the mean temperature, °C; $\bar{T}_{h_0}$ is the mean temperature (°C) at the depth h_0; T_h is the temperature (°C) at a depth h; $\bar{q}$ is the heat flux, kcal/ /hr; I_S is the heat flow from the interior of the earth, kcal/hr; $\alpha = k/\rho c$ is the thermal diffusivity, m^2/hr; k is the thermal conductivity, kcal/m · hr · deg; c is the specific heat, kcal/kg · deg; ρ is the density, kg/ /m^3; L is the latent heat of phase transitions; ν is the geothermal gradient, °C/m; g_0 is the initial geothermal gradient, °C/m; H is the enthalpy of water, kcal/ /kg; $a = k_2\alpha_1^{1/2}/k_1\alpha_2^{1/2}$ and $b = \alpha_1^{1/2}/\alpha_2^{1/2}$, where the subscripts 1 and 2 are for two different melts; $s = k_1\alpha^{1/2}/ /k\alpha_1^{1/2}$; $b_1 = 1 - (p\rho'c'/\rho_0 c_0)(1 - \rho''/\rho')$; ρ' is the density of water, kg/m^3; ρ'' is the vapor density, kg/m^3; c' is the specific heat of water, kcal/kg · deg; $r_1 = = (\alpha_0/\alpha)^{1/2}$; ω is the flow rate of the subsurface water, m^2/hr; $w = \omega c_\omega \rho_\omega / c\rho$; ω is the subscript relating to solution; $\mathrm{tg}\, 2\varphi = 2\pi\alpha/tw^2$; $\gamma = \sqrt[4]{\left(\frac{w}{2\alpha}\right)^4 + \left(\frac{2\pi}{t\alpha}\right)^2}$; A_0 is the amplitude of oscillations of mean temperature $\bar{T}$; t is the period of cyclic variation of T; $p = \omega\nu c/k$; A_{h_0} is the amplitude of temperature oscillations at depth h_0; $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-z^2)\,dz$ is the tabulated error function; $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x)$.

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