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Modeling of a heterophase flow in permeable zones of the lithosphere*

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Abstract. This paper investigates a magma flow in permeable zones of the lithosphere. The model equations describing the dynamics of saturated porous media both without tangential stresses and with them are presented. The phenomenological method used for deriving the equations provides the thermodynamic correctness. Based on the model of the heterophase medium without shear stresses, the conditions under which melting and forming in this magma chambers in such a medium is possible, are analyzed.

1. Introduction

The problem of modeling the evolution of fluid-magmatic systems is important. The dynamics of the convective heat transfer in permeable zones of the continental lithospheric mantle is usually described by means of the Darcy approximation. This approximation is valid in describing the magmatism and associated fluid systems when flows in high-permeability zones are close to stationary regimes. However, studying the minerals structure of the deepest mantle xenoliths indicates to violation of conditions. For the seismic-prone zones of active remote areas of the Pacific ocean this situation is typical not only of the mantle wedge, but also for shear zones in the Earth's crust. Numerical simulation of processes in the lithospheric mantle above astralisms has shown that the melting of mafic magmas in the form of multilevel lesions is possible according to the following scheme: metasomatizing depleted ultrabasic rocks of the lithosphere by flows of above-astonosphera magmatic fluids, introducing Si, Ca, Al, Na, K, followed by the melting of areas of the corresponding structure in the formed sequence of the infiltration metasomatic column. The sequence of multilevel sources corresponds to debasification areas and secondary basification of the original mantle substances.

The description of such systems is possible with the use of more general nonlinear non-stationary models with allowance for the dynamics of heat and mass transfer of multi-component heterogeneous media, the dynamics of rocks deformation in a wide range of temporal and spatial scales.

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This paper proposes the approach involving the joint use of the thermodynamically consistent mathematical model of nonlinear non-stationary dynamics of the heat-mass transfer in heterogeneous media and a non-isothermal model of the flowing multi-reservoir reactor, allowing one to describe the processes of equilibrium metasomatic conversion of the depleted ultrabasic rocks. This approach allows carrying out the physico-chemical analysis of occurring substances whose convective melting may lead to the formation of carbonate, mafic and other magmas. The scheme of the numerical experiments within the non-isothermal model of the flowing multi-reservoir reactor was presented by K.V. Chudnenko [1].

The interaction of rocks and supercritical fluids terms of the schemes of infiltration metasomatism is considered [2]. In such a formulation, the dynamics of the fluid-rock interaction is considered as convective heat and mass transfer with the development of the heterophase equilibrium of chemical reactions in a heterogeneous medium.

The heterophase interaction within the model of the flowing multi-reservoir reactor based on minimization of the Gibbs potential is estimated. The algorithmic implementation of such a harmonization is to ensure that at each time step the heat and mass transfer in a porous medium for the current values of pressure and temperature in a sequential chain of reactors, the problem of calculating the heterogeneous phase equilibrium is solved.

2. The model

The difficulty of experimental verification of the simulation results of fluid-magmatic systems leads to the need of using methods that would generate thermodynamically consistent (which means physically correct) models of the heat and mass transfer. One of the most effective among such methods is the method of conservation laws [3]. This method is based on the coordination procedure of the basic principles of thermodynamics, conservation laws and group invariance of equations thus providing thermodynamically consistent dynamic models of heterogeneous media [4, 5]. The equations of nonlinear dynamics of granular media are built under assumptions of the absence of the phase equilibrium pressure and a small time period of establishing the local thermal equilibrium [6]. The unit volume of a medium, composed of a rock and a fluid (indices $n = 1, 2$, respectively), is characterized by the partial densities of the phases ρ_1, ρ_2, the velocities of the phases $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, the entropy density S. The choice of the energy $E_0 = E_0(\rho_1, \rho_2, \boldsymbol{u}_1 - \boldsymbol{u}_2, S)$ fixes the thermodynamics of a medium. The system of governing equations includes the equation of motion of the phases, the continuity equations and the entropy equation as follows:

$$\frac{\partial \rho_1}{\partial t} + \operatorname{div}(\rho_1 \boldsymbol{u}_1) = \tau^{-1} q, \quad \frac{\partial \rho_2}{\partial t} + \operatorname{div}(\rho_2 \boldsymbol{u}_2) = -\tau^{-1} q,$$

$$
\begin{gathered}
\frac{\partial j_i}{\partial t} + \partial_k(\rho_1 u_{1i} u_{1k} + \rho_2 u_{2i} u_{2k} + p\delta_{ik} - (\varsigma_1 + \varsigma_{12})\delta_{ik} \operatorname{div} \boldsymbol{u}_1 - \\
(\varsigma_2 + \varsigma_{12}\delta_{ik} \operatorname{div} \boldsymbol{u}_2 - (\eta_1 + \eta_{12}) u_{1ik} - (\eta_2 + \eta_{12}) u_{2ik}) = \rho g_i, \\
\frac{\partial u_{2i}}{\partial t} + (\boldsymbol{u}_2, \nabla) u_{2i} = -\frac{1}{\rho}\partial_i p + \frac{\rho_1}{\rho}\partial_i\Big(q + \frac{1}{2}\boldsymbol{w}^2\Big) - \frac{1}{\rho_2} b(j_i - \rho u_{1i}) + \\
\frac{1}{\rho_2}\partial_k(\eta_2 u_{2ik} + \eta_{12} u_{1ik}) + \frac{1}{\rho_2}\partial_i(\varsigma_2 \operatorname{div} \boldsymbol{u}_2 + \varsigma_{12} \operatorname{div} \boldsymbol{u}_1) + g_i, \\
\frac{\partial S}{\partial t} + \operatorname{div}\Big(S\frac{\boldsymbol{j}}{\rho} - 2\lambda\frac{1}{\rho}(\boldsymbol{j} - \rho_1 \boldsymbol{u}_1) - \kappa\frac{1}{T^2}\nabla T\Big) = \frac{R}{T}.
\end{gathered}
$$

The dissipative function R is determined by the ratio

$$
\begin{aligned}
R = {} & \frac{1}{\rho_2} b(j_i - \rho u_{1i})(j_i - \rho u_{1i}) + \kappa\Big(\frac{\nabla T}{T^2}\Big)^2 + \\
& \frac{1}{2}\eta_1 u_{1ik} + \frac{1}{2}\eta_2 u_{2ik} + \eta_{12} u_{1ik} u_{2ik} + \\
& \varsigma_1(\operatorname{div} \boldsymbol{u}_1)^2 + \varsigma_2(\operatorname{div} \boldsymbol{u}_2)^2 + {+}\varsigma_{12} \operatorname{div} \boldsymbol{u}_1 \operatorname{div} \boldsymbol{u}_2 + \tau^{-1} q^2.
\end{aligned}
$$

Here $u_{1ik} = \partial_k u_{1i} + \partial_i u_{1k} - \frac{2}{3}\delta_{ik} \operatorname{div} \boldsymbol{u}_1$, $u_{2ik} = \partial_k u_{2i} + \partial_i u_{2k} - \frac{2}{3}\delta_{ik} \operatorname{div} \boldsymbol{u}_2$, p is the pressure, q is the interfacial interaction parameter, and $\boldsymbol{g}$ is the free fall acceleration. The interfacial kinetic coefficient of friction b, the shear viscosity of phases η_i, the thermal conductivity of the two-phase medium κ, the relaxation time τ and the coefficient ν are the functions of thermodynamic parameters. The equations of state of the two-phase medium

$$
\begin{gathered}
\delta\rho_1 = \rho_1\alpha\,\delta p + \rho_1\rho_2\alpha_q\,\delta q - \rho_1\beta\,\delta T, \quad \delta\rho_2 = \rho_2\alpha\,\delta p - \rho_1\rho_2\alpha_q\,\delta q - \rho_2\beta\,\delta T, \\
\delta s = \frac{c_p}{T}\,\delta T - \frac{1}{\rho}\beta\,\delta p,
\end{gathered}
$$

are obtained in the linear approximation. The volume compression coefficients α, α_q, of the thermal expansion β, of the specific heat c_p, were taken additive with respect to subsystems.

This system of equations of the two-velocity hydrodynamics of a viscous fluid-saturated granular medium describes a two-phase medium, which in shear stresses is not considered. If a substance, containing a large enough number of solid particles, is moving along magma channels, or if the porosity of weakened zones of the lithosphere is taken into account, there appears a need of considering elastic properties of a porous matrix. In this case, the equations of motion of fluid-saturated porous media, with allowance for the shear stresses are supplemented by the equation for the metric deformations tensor g_{ik} [4, 5]:

$$\frac{\partial \rho_1}{\partial t} + \operatorname{div}(\rho_1 \boldsymbol{u}_1) = \tau_b^{-1} h_{ll}, \quad \frac{\partial \rho_2}{\partial t} + \operatorname{div}(\rho_2 \boldsymbol{u}_2) = -\tau_b^{-1} h_{ll},$$

$$\frac{\partial g_{ik}}{\partial t} + (\boldsymbol{u}, \nabla) g_{ik} + g_{in}\partial_k u_n + g_{in}\partial_n u_k = -\tau_s^{-1} g_{in}(h_{nk} - h_{ll}\delta_{nk}),$$

$$\frac{\partial j_i}{\partial t} + \partial_k \Big(\rho_1 u_{1i} u_{1k} + \rho_2 u_{2i} u_{2k} + p\delta_{ik} + h_{in} g_{nk} - (\varsigma_1 + \varsigma_{12})\delta_{ik} \operatorname{div} \boldsymbol{u}_1 -$$
$$(\varsigma_2 + \varsigma_{12})\delta_{ik} \operatorname{div} \boldsymbol{u}_2 - (\eta_1 + \eta_{12}) u_{1ik} - (\eta_2 + \eta_{12}) u_{2ik}\Big) = \rho g_i,$$

$$\frac{\partial u_{2i}}{\partial t} + (\boldsymbol{u}_2, \nabla) u_{2i} = -\frac{1}{\rho}\partial_i p + \frac{\rho_1}{2\rho}\partial_i \boldsymbol{w}^2 - \frac{1}{2\rho} h_{in}\partial_i g_{nk} - \frac{1}{\rho_2} b(j_i - \rho u_{1i}) +$$
$$\frac{1}{\rho_2}\partial_k(\eta_2 u_{2ik} + \eta_{12} u_{1ik}) + \frac{1}{\rho_2}\partial_i(\varsigma_2 \operatorname{div} \boldsymbol{u}_2 + \varsigma_{12} \operatorname{div} \boldsymbol{u}_1) + g_i,$$

$$\frac{\partial S}{\partial t} + \operatorname{div}\left(S \frac{}{j}\rho - 2\lambda \frac{1}{\rho}(\boldsymbol{j} - \rho_1 \boldsymbol{u}_1) - \kappa \frac{1}{T^2}\nabla T\right) = \frac{R}{T}.$$

The dissipative function R takes the form

$$R = \frac{1}{\rho_2} b(j_i - \rho u_{1i})(j_i - \rho u_{1i}) + \kappa \Big(\frac{\nabla T}{T^2}\Big)^2 +$$
$$\tau_s^{-1} g_{in}(h_{nk} - h_{ll}\delta_{nk}) g_{im}(h_{mk} - h_{ll}\delta_{mk}) + \tau_b^{-1}(h_{ll})^2 +$$
$$\frac{1}{2}\eta_1 u_{1ik} + \frac{1}{2}\eta_2 u_{2ik} + \eta_{12}\partial_k u_{1ik}\partial_k u_{2ik} +$$
$$\varsigma_1(\operatorname{div} \boldsymbol{u}_1)^2 + \varsigma_2(\operatorname{div} \boldsymbol{u}_2)^2 + \varsigma_{12} \operatorname{div} \boldsymbol{u}_1 \operatorname{div} \boldsymbol{u}_2 + \tau^{-1} q^2.$$

The interfacial friction kinetic coefficient b, the tangential stresses relaxation τ_s, the relaxation time τ_b, the shear viscosity of phases η_i, the thermal conductivity of the two-phase medium κ and the coefficient ν are also the functions of the thermodynamic parameters.

Further, the dependence of the energy on the shear deformations will be neglected.

3. Statement of the problem

In this paper, the problem of the filtration fluid flow in a permeable zone in the lithospheric statement and the problem of describing the evolution of the mineral composition as a result of accompanying interactions of the fluid with the rock are investigated [10]. We consider a rectangular computational domain with the characteristic dimensions $L_x = 4$ km, $L_y = 100$ km.

At the initial time instant a linear temperature profile in the range 130–1330°C is set along the computational domain. At the lower boundary the temperature is fixed: at the lateral boundaries the temperature difference of the host rocks between the upper and the lower boundaries

Table 1. The physical parameters of the phases used in the calculations of the filtration flow tectonic fluid in the permeable zone

Physical parameters	Solid phase	Liquid phase
ρ, kg/m^3	2600	550
α, Pa^{-1}	$3.2 \cdot 10^{-13}$	$9.5 \cdot 10^{-10}$
β, K^{-1}	$7.0 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$
η_r, kg/(m·s)	$1.0 \cdot 10^{18}$	$4.5 \cdot 10^{-5}$
ξ, m^2/s	$7.7 \cdot 10^{-7}$	$7.7 \cdot 10^{-7}$

Table 2. The structure of the permeable zone

Depth, km	Liquid volume fraction	Darcy number
0–10	0.03	$1.0 \cdot 10^{-21}$
10–20	0.03	$1.0 \cdot 10^{-21}$
20–40	0.025	$3.0 \cdot 10^{-22}$
40–60	0.025	$1.0 \cdot 10^{-22}$
40–80	0.02	$3.0 \cdot 10^{-23}$
80–100	0.02	$3.0 \cdot 10^{-24}$

of the computational domain 30–680°C and the heat transfer coefficient $k = 0.001$ W/(m^{2}K) is specified.

The calculations were carried out for the two-phase medium with the physical parameters of phases (Table 1), corresponding to the rock granites type (the first solid phase) and the lithospheric fluid (the second liquid phase) in the channel of a layered structure from distributions of the volume fraction of the fluid phase and the Darcy number (Table 2, Figure 1). The velocity of the liquid phase at the lower boundary of the computational domain is equal to $u_{2y} = 10^{-6}$ m/s.

The dynamics of such a medium is described by the system of dimensionless equations [12]:

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i \boldsymbol{u_i}) = 0, \quad i = 1, 2,$$

$$\frac{\partial(\rho s)}{\partial t} + \operatorname{div}((\rho_1 \boldsymbol{u}_1 + \rho_2 \boldsymbol{u}_2)s) = \frac{1}{T+H}\Delta T + \frac{1}{T+H}\mathrm{ND}\frac{1}{\rho_0}\mathrm{DaPr}_2\frac{\rho_2}{\rho}(\boldsymbol{u}_1 - \boldsymbol{u}_2)^2,$$

$$\frac{\partial(\rho_i \boldsymbol{u_i})}{\partial t} + (\rho_i \boldsymbol{u_i}, \nabla)\boldsymbol{u_i} = \frac{1}{\rho_0}\mathrm{DaPr}_i \Delta \boldsymbol{u_i} - \frac{\rho_i}{\rho}\nabla P + (-1)^i \frac{\rho_1 \rho_2}{\rho}\nabla Q + (-1)^i \frac{1}{\rho_0}\mathrm{DaPr}_i \frac{\rho_2}{\rho}(\boldsymbol{u}_1 - \boldsymbol{u}_2) + \boldsymbol{e}_i \cdot \mathrm{Ra}_i \mathrm{Pr}_i \rho_i.$$

This system is characterized by the following dimensionless parameters:

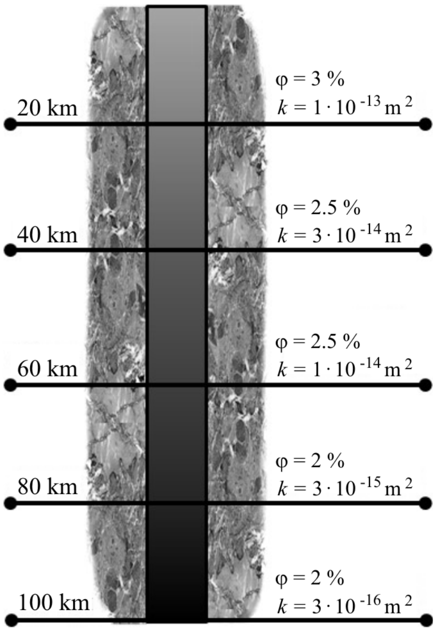

Figure 1. The scheme of the permeable zone structure

Rayleigh $\mathrm{Ra}_i = \frac{gL^3}{\chi\nu_i}$, Prandtl $\mathrm{Pr}_i = \frac{\nu_i}{\chi}$, Darcy $\mathrm{Da} = \frac{L^2}{k}$, and $\mathrm{ND} = \frac{\chi^2}{c_p \Delta T L^2}$.

At the lateral boundaries, the boundary conditions of non-flowing and adhesion are set:

$$u_{1x}|_{x=0} = u_{1y}|_{x=0} = 0$$

and, similarly, for the velocity vector components of the second phase and at the lateral boundary $x = L_x$ of the computational domain.

At the lower (input) boundary of the computational domain, two types of boundary conditions are admissible: 1) the velocity of the input flow is set as follows:

$$u_{1x}|_{y=0} = u_{1x(\mathrm{in})}, \quad u_{1y}|_{y=0} = u_{1y(\mathrm{in})},$$

and, similarly, for the velocity vector components of the second phase; 2) the value of the pressure parameter of the interfacial interaction:

$$P|_{y=0} = P_{(\mathrm{in})}, \quad q|_{y=0} = q_{(\mathrm{in})},$$

and conditions for the velocities:

$$\left.\frac{\partial u_{1x}}{\partial y}\right|_{y=0} = 0, \quad \left.\frac{\partial u_{1y}}{\partial y}\right|_{y=0} = 0,$$

and, similarly, for the velocity vector components of the second phase

At the upper (output) boundary of the computational domain, the conditions for the pressure and the interfacial interaction parameter are set:

$$\left.\frac{\partial P}{\partial y}\right|_{y=L_y} = 0, \quad \left.\frac{\partial q}{\partial y}\right|_{y=L_y} = 0,$$

and conditions for the velocities:

$$\left.\frac{\partial u_{1x}}{\partial y}\right|_{y=L_y} = 0, \quad \left.\frac{\partial u_{1y}}{\partial y}\right|_{y=L_y} = 0,$$

and, similarly, for the velocity vector components of the second phase.

The calculated time step is $\Delta t = 1$ year, the mesh size is 20×200 nodes.

For the numerical solution of the problem posed we have used an algorithm based on the control volume method [12, 11]. Discrete analogs to the differential equations derived for this method contain the exact integral conservation of such values as mass, total momentum and energy. The implicit time-discrete analog was used, which is necessary for the ability of counting at arbitrary time scales. The SIMPLE algorithm for the calculation of consistent fields of the pressures in the phases and in the phase velocities has been adapted. A specific feature of the implementation of this algorithm takes into the account the compressibility of the phases, thus providing a steady count in the extreme thermodynamic conditions.

4. The results of modeling

In this paper we present the results of the numerical modeling of the convective heat and mass transfer that are taken into account when modeling the dynamics of the equilibrium infiltration metasomatism, not accompanied by partial or complete melting of some zones in the metasomatic column.

Figure 2a–c presents the results of calculations performed with the non-equilibrium in pressure two-velocity model of compressible two-phase media, reflecting the dynamics of the fields, the vertical components of the velocity vector of the liquid phase, pressure and temperature needed for the subsequent geochemical analysis using the Program Selector [1]. The values of the following variables at the points located along the Central vertical section of the computational domain are transferred to the multi-reservoir model: temperature, pressure, the vertical component of the velocity vector of the liquid phase, the mass flow of the liquid phase through the horizontal section of the calculation domain per time unit.

It should be noted that in the above-mentioned approach, the equations of physico-chemical dynamics of metasomatic transformations of rocks of the lithospheric mantle based on the model of heterophase interaction "fluid-breed" was used in the hydraulic approximation [13]. However, such a simplification leads to a rapid achievement of the steady state of a flow of fluid in the rock and gives underestimated values of the time evolution of such systems. The obtained fields of temperature and pressure in the permeable zone in the presented, more general model, differ from those obtained in [13] in a substantially higher pressure in the fluid in the section, significantly slower temperature rise and the thermal front motion associated with the energy absorption and heat release due to the interfacial friction.

The combination of hydrodynamics with a magmatic source and petrogenic components in the model [1] allows one to reveal specific features of the dynamics of the fluid-rock interactions in the two-layer mantle-crust fluid systems. Figure 3 shows significant differences in the distribution of

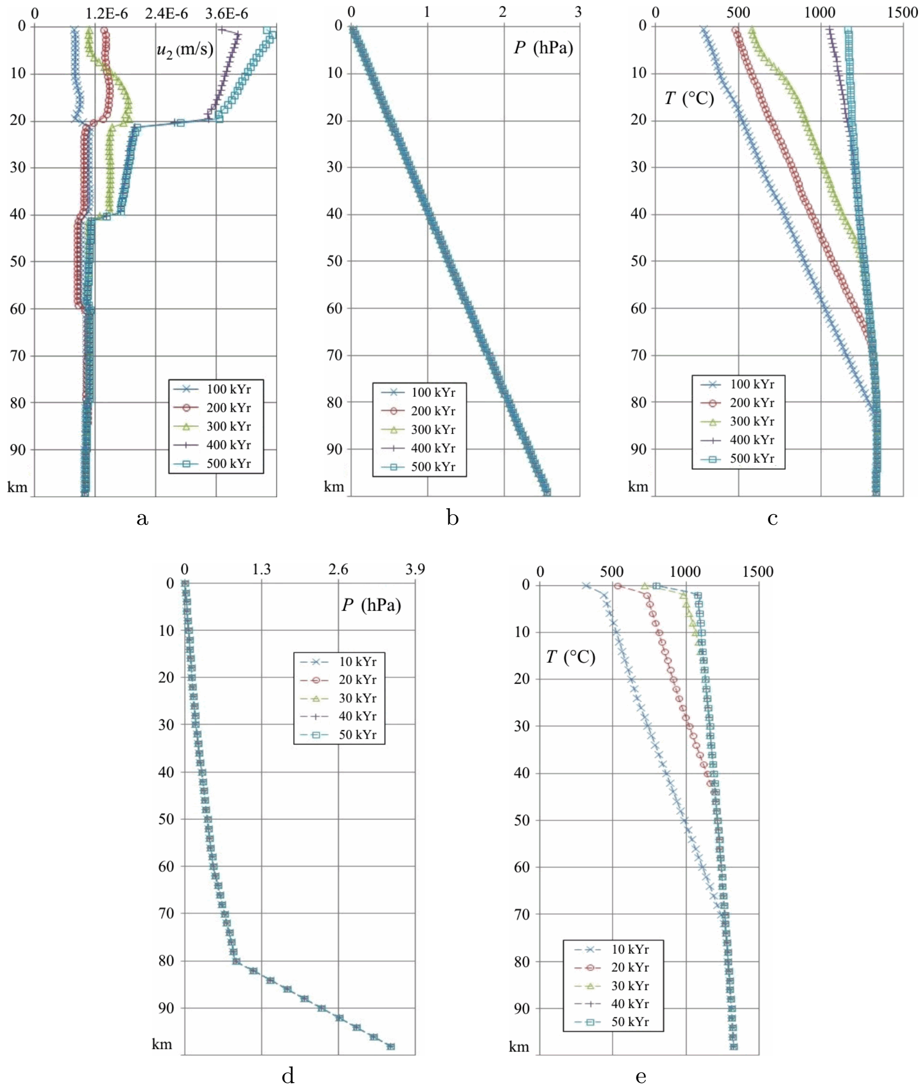

Figure 2. The time evolution of the resulting parameters of the filtration flow of the lithospheric fluid in the permeable zone along the Central vertical section of the calculation domain with the non-equilibrium pressure model of compressible two-phase media: a) the vertical components of the velocity vector of the liquid phase, b) pressure, and c) temperature; in the one-velocity Darcy's approximation of d) pressure and e) temperature

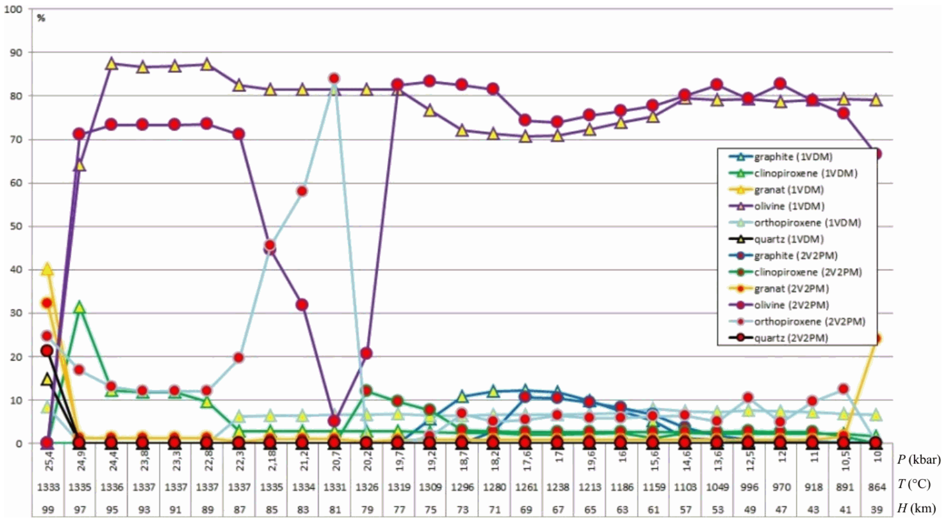

Figure 3. Distribution of the mineral composition along the permeable zone according to the geochemical analysis (Selector), based on the hydrodynamic modeling in the two-phase model (2V2PM) and the one-velocity model (1VDM)

the mineral composition along the permeable zone, obtained by the geochemical analysis (using Selector), the results of hydrodynamic modeling in the proposed model of compressible two-phase media in the one-velocity Darcy's approximation [13]. The wehrlification zones ($T > 1000$°C) that are valid for the initial temperature distribution completely disappear with the thermal front motion in the two-velocity model being replaced by higher-temperature mineral associations. Moreover, the existence of a specified internal heat source can be a determining factor both for the development of specific zoning and the development of intermediate sources of melting in the lithosphere.

5. Geological implications

At the quasi-stationary stage of the evolution of the fluid system, the temperature distribution in the lower part of the conductor, the temperature (depending on the values of effective permeability) is always higher than in the fluid source by the factor of ten up to hundreds degrees.

Therefore, when analyzing the dynamics of metasomatic processes correctly it is possible to investigate the temperature range with which the development of melting in some areas of the arising column is not expected. Since this issue has been adequately investigated in the study of the dynamics of carbonatization [14], in the numerical experiments, the temperatures in the metasomatic column were limited to the interval 1300–1340°C.

We have investigated the types of metasomatic columns with the fluid temperature variation in the magmatic source from 1100 to 1330°C for AC and DC content of petrogenic components in the molar ratio of contents of independent components of the fluids source: from C(1), N(0.01). The variation of the molar quantities of petrogenic components in the fluid was in agreement with the previously defined area of harzburgites wehrlitization.

The differences in the dynamics of the development of metasomatic zoning for one- and two-velocity models in the fluid systems of the lithospheric mantle are reduced to a much greater period of formation of the metasomatic zones, to the facial differences in the composition and in the ratios of the mineral associations that are related to an increase of pressure in the fluid system.

The observed differences: at pressures above 20 kbar for the temperatures below 1150°C the rate of synthesis of clinopyroxene with the same intensity of decomposition of olivine is about two times as large as orthopyroxene. Thus, in the fluid system, in the wehrlitization in the high-temperature zones, the contents of orthopyroxene in associations is higher than in the upper half of arising metasomatic columns.

At the temperature $T < 1300$°C a number of mineralogical effects related to variations of the fluid composition in the source are revealed: 1) for different relations of the contents of Si/Ca in a fluid, debasification of ultrabasites are implemented with geological ranges of the compositions of metasomatic rocks from carbonatites to gracedieus; 2) complete replacement of olivine by orthopyroxene at ≈ 975°C.

For the case $T \geq 1330$°C, anomalous wehrlitization development for the range of ratios in the fluid $1 \leq \mathrm{Si/Ca} \leq 5$ has been revealed.

6. Conclusion

The approach to a correct mathematical description of the mantle-crustal magmatogene fluid system has been proposed. There is shown a possibility of the occurrence in the fluid systems of the three levels of changes in the mineral composition of the original depleted ultrabasites, where manifestations of the melting zones with the formation of mafic liquids are possible. In the lower part of the Earth's crust the heating temperatures can attain values that would be necessary for the melting of granitoid magmas, and for the development of granitization, i.e. the appearance of granitic melts.

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