Global Journal of Researches in Engineering: I
Numerical Methods
Volume 20 Issue 1 Version 1.0 Year 2020
Type: Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals
Online ISSN: 2249-4596 & Print ISSN: 0975-5861

Application of Numerical Methods for New Estimate of Rheology Constants in the 2D Computer Model of the Mantle Wedge Thermal Convection as a Possible Physical Mechanism of Hydrocarbons Transport

By S.V.Gavrilov & A.L.Kharitonov

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GJRE-I Classification: FOR Code: 090408

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S.V.Gavrilov [α] & A.L.Kharitonov [σ]

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I. Introduction

Interaction of the lithospheric plates in the Crimea-Caucasus region leads to the thrusting of the Black Sea micro-plate under the Crimea peninsula (under the Scythian plate) [Nimetulayeva, 2004]. As a consequence, the seismic focal plane is formed along which the Crimea ascends as the result of seismic jerks. The velocities of vertical uplift of the Crimea mountains and sinking of the near-Crimean area of the Black Sea micro-plate equal to ~4 mm per year and ~10 mm per year, respectively. Mountainous Crimea is a folded fault region being a part of the Alps-Himalaya-Indonesia belt [Yudin, 2001].

Author α: Schmidt Institute of Physics of the Earth, Russian Academy of Sciences, RAS, Troitsk, RF.

Author σ: Pushkov Institute of Terrestrial Magnetism, Ionosphere and Radio Wave Propagation, RAS, Troitsk, RF. e-mail: ahariton@izmiran.ru

In [Ushakov et al., 1977] the subduction velocity of the Black Sea micro-plate under the Crimea peninsula is estimated of ~1 mm per year as the best fit to the observed sedimentary layer distribution. Other estimations are unknown to the knowledge of the authors. However the obtained estimate of ~1 mm per year appears to be an underestimate, being not correspondent to the vertical velocities of ~4 and ~10 mm per year of Mountainous Crimea and the Black Sea micro-plate.

According to [Gavrilov, 2014; Gerya, 2011; Gerya et al., 2006] two types of dissipation driven small-scale thermal convection in the mantle wedge are possible, viz. 3D finger-like convective jets, raising to volcanic chain, and 2D transversal Karig vortices, aligned perpendicularly to subduction. These two types of convection are shown to be spatially separated due to the pressure and temperature dependence of mantle effective viscosity, the Karig vortices, if any of them formed, being located behind the volcanic arc [Gavrilov, 2014]. Despite the firmly established localization of the seismic focal plane there is just a single definite conclusion concerning the velocity of subduction of the Black Sea micro-plate [Ushakov et al., 1977]. It is not completely clear if volcanism played a substantial role in forming Mountainous Crimea, or the mountains are of a purely thrust-and-fold origin. [Nimetulayeva, 2004] indicates the contradictory statements on the Crimean volcanism to have been published, however in Fig.2.4 in [Nimetulayeva, 2004], the volcanic eruption in the Mountainous Crimea is depicted. The abovementioned picture is reproduced here in Fig.1 with the convective vortices drawn additionally. It is worth assuming the two heat flux anomaly maxima observed in the south of the Crimea peninsula [Smirnov, 1980; Nimetulayaeva, 2004, Fig.2.4] owe their origin to respectively 3D and 2D upward convective heat transfer from the mantle wedge to the Earth's surface (see Fig.1 of this paper). The latter 2D maximum located in the rear of the Mountainous Crimea is much greater as compared to the former 3D maximum located in the Mountainous Crimea. The 2D

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heat flux anomaly maximum is associated with the 2D upward convective flow in the mantle wedge. Numerical modeling of 2D mantle wedge thermal convection occurring in the form of the Karig vortices and presumably transporting heat to the Earth's surface in the rear of the Mountainous Crimea allows judging about the mean velocity of subduction of the Black Sea micro-plate under the Crimea peninsula as well as about the rheological mantle parameters. The horizontal extent of the 2D heat flux anomaly in the rear of the Mountainous Crimea is shown to correspond to the mean subduction velocity >10 mm per year for the observed subduction angle 15°. Numerical convection models accounting for the effects of phase transitions as well as the pressure, temperature, and viscous stresses viscosity dependence fit in well with the heat flux observational data in the case of non-Newtonian mantle rheology at the mean concentration of water in the mantle wedge of ~1 wt. %.

II. Algorithm and Computation Complexity

Thermo-mechanical model of the mantle wedge between the base of the overlying Scythian plate and the upper surface of the Black Sea micro-plate subducting under the Scythian one with a velocity V at an angle β is obtained for the infinite Prandtl number fluid as the solution of non-dimensional 2D hydrodynamic equations in the Boussinesq approximation for the stream-function ψ and temperature *T*.

$$(\partial_{zz}^2 - \partial_{xx}^2)\eta(\partial_{zz}^2 - \partial_{xx}^2)\psi + 4\partial_{xz}^2\eta\partial_{xz}^2\psi = RaT_x - Ra^{(410)}\Gamma_x^{(410)} - Ra^{(660)}\Gamma_x^{(660)}, \quad (1)$$

$$\partial_t T = \Delta T - \psi_z T_x + \psi_x T_z + \frac{Di}{Ra} \times \frac{\tau_{ik}^2}{2\eta} + Q, \quad (2)$$

Here η is dynamic viscosity, ∂ and indices denote partial derivatives with respect to coordinates x (horizontal), z (vertical) and time t, Δ is the Laplace operator, $\Gamma^{(410)}$ and $\Gamma^{(660)}$ are volume ratios of the heavy phase at the 410 km and 660 km phase boundaries, the velocity components V_x and V_z are expressed through ψ as

$$V_x = \psi_z, \; V_z = -\psi_x, \quad (3)$$

while non-dimensional Rayleigh number Ra, phase numbers $Ra^{(410)}$, $Ra^{(660)}$ and dissipative number Di are

$$Ra = \frac{\alpha\rho g d^3 T_1}{\bar{\eta}\chi} = 5.55\times10^8, \quad Ra^{(410)} = \frac{\delta\rho^{(410)} g d^3}{\bar{\eta}\chi} = 6.6\times10^8,$$

$$Ra^{(660)} = \frac{\delta\rho^{(660)} g d^3}{\bar{\eta}\chi} = 8.5\times10^8, \quad Di = \frac{\alpha g d}{c_p} = 0.165, \quad (4)$$

where α =3·10^{-5} K^{-1} is the thermal expansion coefficient, ρ =3.3 g·cm^{-3} is the density, *g* is gravity acceleration, c_p = 1.2×10^3 J · kg^{-1}K^{-1} is specific heat capacity at constant pressure, T_1 = 1950 K is the temperature at the base of the mantle transition zone (MTZ) at depth 660 km regarded the lower boundary of the model domain, *Q*= 6.25·10^{-4} mW·m^{-3} is the volumetric heat generation in the crust, τ_{ik} is the viscous stress tensor, *d*=660 km is the vertical dimension of the modeled domain, $\bar{\eta}$ = 10^{18} Pa · s is the viscosity scaling factor, χ =1 mm^2 · s^{-1} is thermal diffusivity, $\delta\rho^{(410)} = 0.07\rho$ and $\delta\rho^{(660)} = 0.09\rho$ are the density changes at the 410 km and 660 km phase boundaries respectively. In (1), (2) the scaling factors for time *t*, coordinates x and z, stresses τ_{ik}, and the stream-function ψ are $d^2 \cdot \chi^{-1}$, *d*, $\bar{\eta}\chi \cdot d^{-2}$, and χ respectively. Assuming rheology be linear for the diffusion creep deformation mechanism dominating in the mantle at depths over ~200 km [Billen & Hirth, 2005], we accept the temperature- and lithostatic pressure *p* dependent viscosity as [Zharkov, 2019]

$$\eta = \frac{\mu}{2A}\left(\frac{h}{b^*}\right)^m \exp\frac{E^* + pV^*}{RT}, \tag{5}$$

Where for "wet" olivine A=5.3×10^15 s^-1, m=2.5, the grain size h =10^-1 – 10 mm, b^*=5×10^-8 cm is the Burgers vector [Zharkov, 2003], E^*=240 kJ·mol^-1 is activation energy, V^*=5×10^3 mm^3·mol^-1 is activation volume, μ =300 GPa is the shear modulus normalizing factor, R is the gas constant. At the chosen constants and the grain size h=1.6 mm, non-dimensional viscosity also denoted η is

$$\eta = 5.0\times10^{-7}\exp\frac{14.8 + 6.72(1-z)}{T}, \tag{6}$$

Where T is non-dimensional temperature, non-dimensional z normalized by d is pointing upwards from the MTZ base and x is pointing against subduction along the MTZ base. The aspect ratio of the model domain is 1:3.7 thus the subduction angle being $\beta \approx 15^{\mathrm{o}}$ if subduction is assumed to take place along the model domain diagonal. Non-dimensional trial subduction velocity V=45 mm·a^-1 normalized by $\chi \cdot d^{-1}$ equals V=0.938·10^3, i.e. non-dimensional velocity components of subducting Black Sea micro-plate are V_x = – 0.898·10^3 and V_z = –0.268·10^3.

To check as to how the estimate of the velocity of subduction of the Black Sea micro-plate is sensitive to the accepted linear rheological law here we make extra computations for non-Newtonian rheology, in which case the viscosity formulae (5)–

$$\eta = \frac{1}{2AC_w^r\tau^{n-1}}\left(\frac{h}{b^*}\right)^m \exp\frac{E^* + pV^*}{RT}, \tag{7}$$

Where according to [Trubitsyn, 2012] for "wet" olivine n=3, r=1.2, m=0, $\boxed{\tau = (\tau_{ik}^2)^{1/2}}$, E^*=480 kJ·mol^-1, V^*=11×10^3 mm^3·mol^-1, A=10^2 c^-1×(MPa)^-n, C_w >10^-3 for "wet" olivine is the weight water concentration (in %%). It should be noted the constants in (7) vary considerably in the papers referred to by [Trubitsyn, 2012] and heretofore, we gave averaged values of constants.

At C_w =10^-3 on accounting for

$$\tau_{ik}^2 = 4\eta^2[(\psi_{zz}-\psi_{xx})^2/2 + 2\psi_{xz}^2] \tag{8}$$

non-dimensional viscosity is

$$\eta = \frac{1.00}{[(\psi_{zz}-\psi_{xx})^2/2+2\psi_{xz}^2]^{1/3}}\times\exp\frac{10.0+5.0\times(1-z)}{T}. \tag{9}$$

Following [Trubitsyn & Trubitsyn, 2014] we assume the phase functions $\Gamma^{(l)}$ as

$$\Gamma^{(l)} = \frac{1}{2}\left(1 - th\frac{z - z^{(l)}(T)}{w^{(l)}}\right),\ z^{(l)}(T) = z_0^{(l)} - \frac{\gamma^{(l)}}{\rho g}(T - T_0^{(l)}), \tag{10}$$

where the signs are changed as z-axis is pointing upwards, $z^{(l)}(T)$ is the depth of the l-th phase transition (l=410, 660), $z_0^{(l)}$ and $T_0^{(l)}$ are the averaged depth and temperature of the l-th phase transition, $\gamma^{(410)}$ = 3 MPa×K^-1 and $\gamma^{(660)}$ = –3 MPa×K^-1 are the slopes of the phase equilibrium curves, $w^{(l)}$ is the characteristic thickness of the l-th phase transition, $T_0^{(410)}$ =1800 K, $T_0^{(660)}$ =1950 K are the mean

mean phase transition temperatures. The heats of phase transitions are neglected in (2) as insignificant in the case of developed convection as in [Trubitsyn & Trubitsyn, 2014]. From (10) it follows

$$\Gamma_x^{(l)} = -\frac{\gamma^{(l)}}{2\rho g w^{(l)}} ch^{-2}\frac{z - z_0^{(l)} + \gamma^{(l)}(T - T_0^{(l)})/\rho g}{w^{(l)}} \times T_x, \quad (11)$$

Where from it is clear the phase transition with $\gamma^{(l)} > 0$ facilitates convection (at l=410), while the phase transition with $\gamma^{(l)} < 0$ hinders convection (at l=660). In non-dimensional form $z_0^{(410)}$ =0.38, $z_0^{(660)}$ =0, $w^{(l)}$ =0.05, $\gamma^{(410)}$ =2.5×10⁹, $\gamma^{(660)}$ = –2.5×10⁹, $T_0^{(410)}$ = 0.92, $T_0^{(660)}$ =1, and in (1).

$$\Gamma_x^{(l)} = -\frac{\delta\rho^{(l)}}{\rho Ra^{(l)}}\frac{\gamma^{(l)}}{2w^{(l)}} ch^{-2}\frac{z - z_0^{(l)} - \gamma^{(l)}\dfrac{\delta\rho^{(l)}}{\rho Ra^{(l)}}(T - T_0^{(l)})}{w^{(l)}} \times T_x. \quad (12)$$

Equations (1)–(2) are solved for the isothermal horizontal and insolated vertical boundaries regarded no-slip impenetrable ones except for the "windows" for in- and outgoing subducting plate, where the plate velocity is specified. Vertical boundary distant from subduction zone is assumed penetrable at right angle, the latter boundary condition appears not too imposing in the case of very flat subduction. Q in (2) is non-zero in the continental and oceanic crust 40 and 7 *km* thick. Initial vertical boundaries temperature is calculated for the half-space cooling model for 10^9 yr and 10^8 yr for Scythian (continental) and Black Sea (oceanic) plates respectively.

III. Results and Discussion

Assuming the second (more remote from the trench) heat flux q maximum in Fig.1 appears above the convective flow, ascending to C_2 point in Fig.1, and the convection cell dimension is equal to the two adjacent q minima separation (i.e. the q minima are located above the descending convective flows) we can estimate the convection cell dimension as ~250 km.

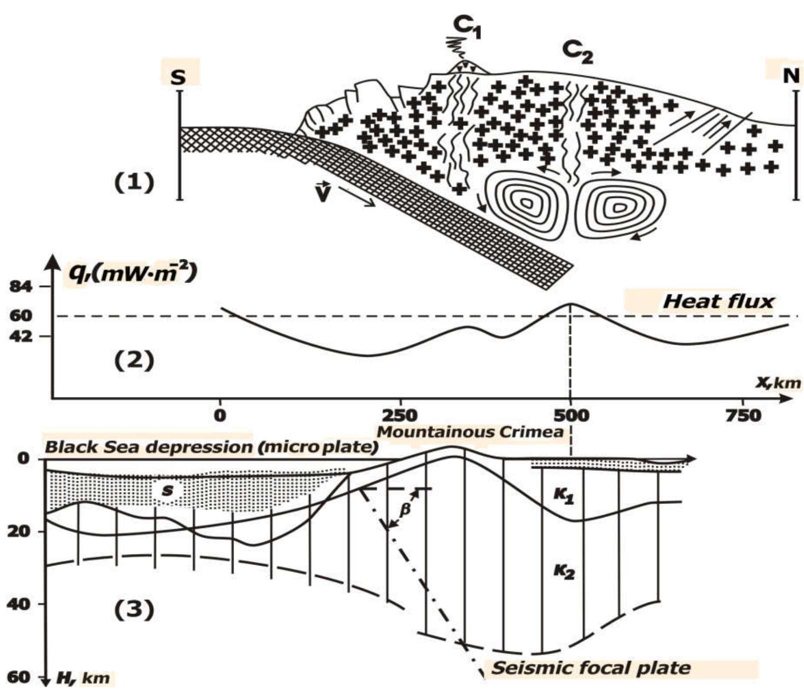

Fig. 1: Schematic cross section of the region of subduction of the Black Sea micro-plate under the Crimea peninsula (Scythian plate) C_1 and C_2 are the zones of 3D and 2D convective flows ascending to the heat flux q maxima, the whirls under C_2 are the 2D Karig convective flows. (2) – Heat flux q in the south of Crimea. (3) – The Black Sea micro-plate subducting under the Crimea peninsula and the seismic focal plane shown by the dotted line. (After [Nimetulayeva, 2006]).

To preliminarily access the mean velocity of subduction of the Black Sea micro-plate the coordinate x dependence of the growth rate $\gamma_{\perp}(x)$ of transversal convective rolls for the constant viscosity fluid model can be allowed for. In such the model the averaged temperature and pressure viscosity dependence is accounted for in an averaged manner, the factor describing the temperature- and pressure viscosity dependence being equal to its mean value [Gavrilov, 2014].

Analytical formulae in [Gavrilov, 2014] yield $\gamma_{\perp}(x)$ shown in Fig.2 for the subduction angle $\beta \approx 15^{o}$, convection cell dimension ~250 km and subduction velocities *V* given in Fig.2 in mm per year.

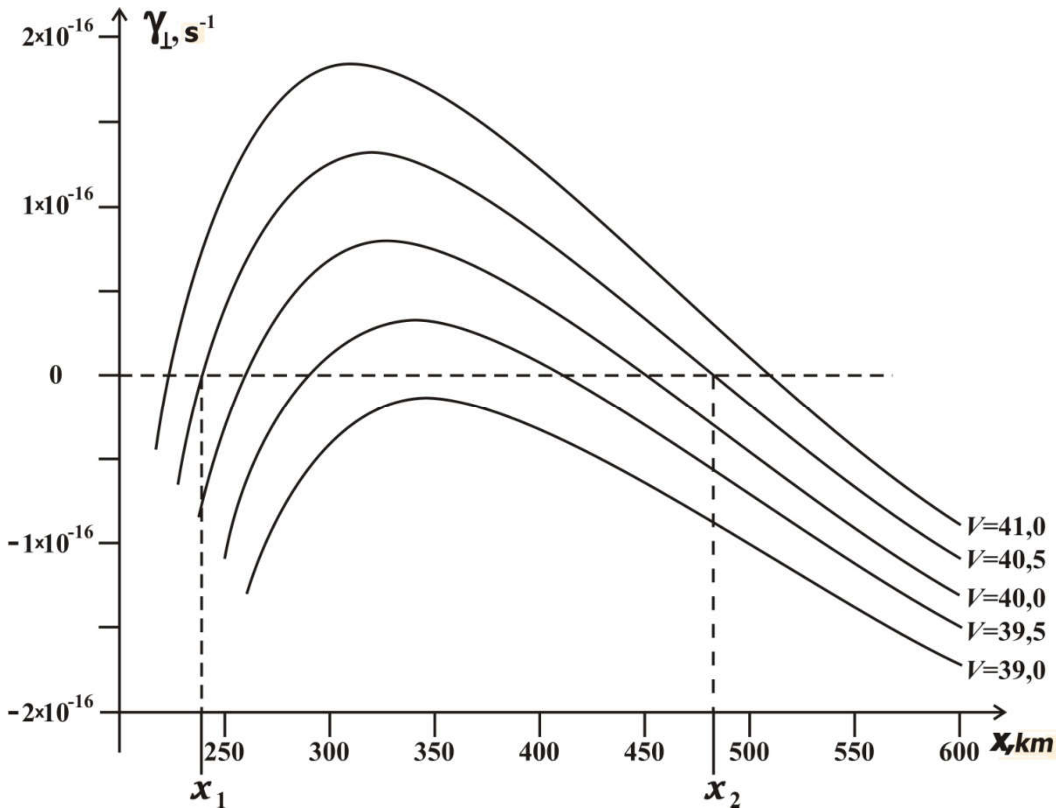

Fig. 2: Growth rate $\gamma_{\perp}(x)$ of convective instability vs. horizontal distance x for subduction velocities *V* in mm per year. In the zone $x_1 < x < x_2$ approximately 250 km long single 2D convection cell with $\gamma_{\perp}(x)>0$ is aroused at V=40.5 mm$\times$yr^{-1} in the zone of heat flux maximum.

It should be noted the growth rates $\gamma_{\perp}(x)$ are viscosity independent as convection is driven by viscous heat release (which is directly proportional to viscosity), while, on the other hand, the greater is the viscosity the more difficult is to arouse the convection. Fig.2 clearly demonstrates the convective zone with $\gamma_{\perp}(x)>0$ amounts to $x_2 - x_1 \approx$250 km (i.e. the single convective cell of ~250 size is actually aroused) at V=40.5 mm per year, the latter value being a preliminary estimate of the mean subduction velocity. The $\gamma_{\perp}(x)$ maximum is ~320 km distant from the trench which is very close to the distance from the trench to the observed 2D heat flux anomaly (~400 km, see Fig.1).

To compute more accurate consistent model of small-scale convection in the mantle wedge between the overriding Scythian plate and subducting Black Sea micro-plate it is necessary from the computational point of view first to specify vanishing non-dimensional numbers $Ra \to 0$, $Di = 0$ in (1)–(2), i.e. to ignore convection and viscous dissipation. This approach is applied as convection with Ra and Di (4) passes through very vigorous stages, and the time steps in integrating (1)–(2) become too small thus making it difficult to model the thermal structure of the plates. Solving (1)–(2) by the finite element method in space on the grid 104$\times$104 and the 3-rd order Runge-Kutta method in time one obtains for $Ra \to 0$, $Di = 0$ and V=45 mm a year non-dimensional quasi steady-state Ψ and T shown in Figs.3, where the streamlines are depicted with step 0.25 and the isotherms with an interval of 0.05.

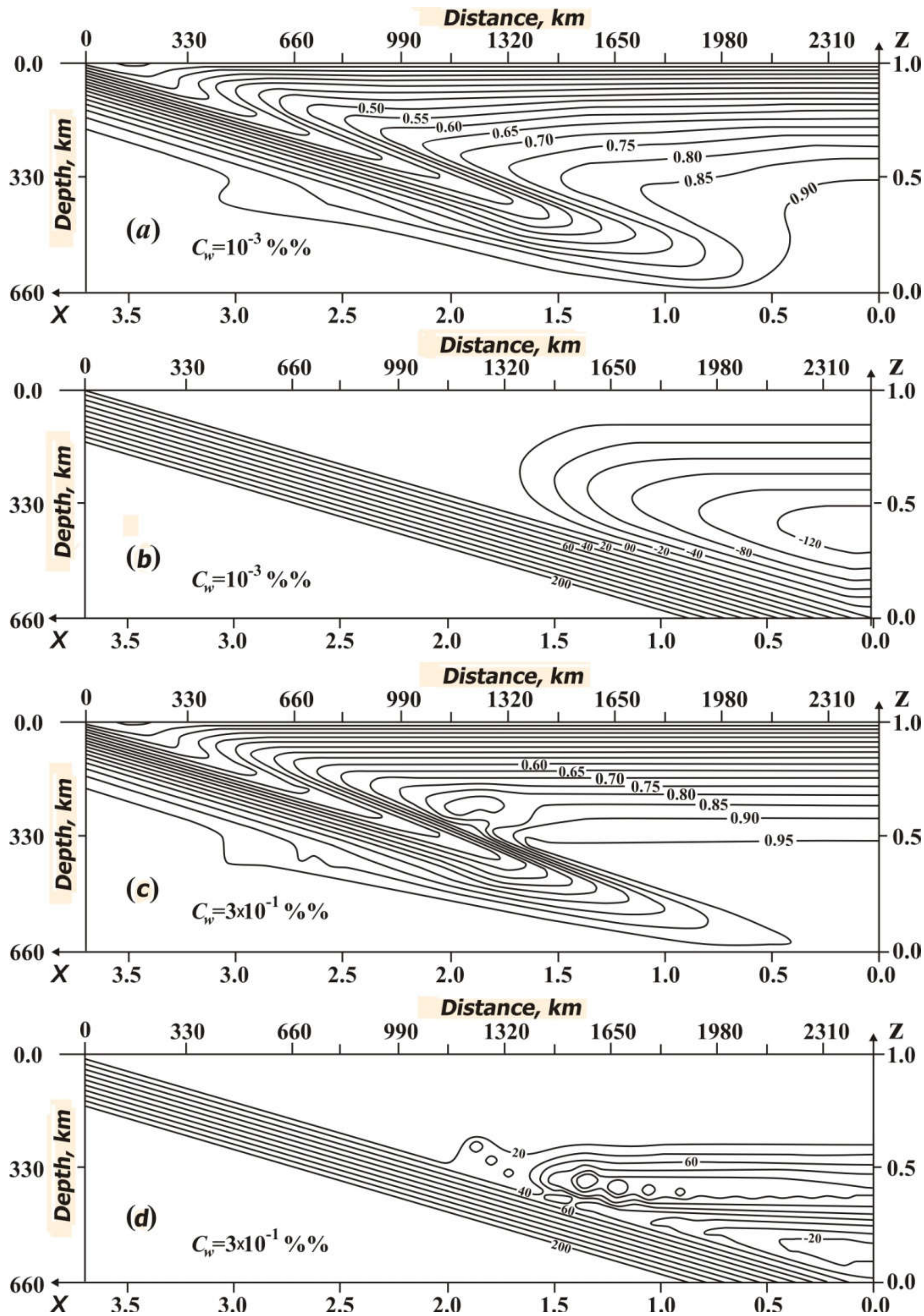

Fig. 3: Quasi steady-state non-dimensional stream-function and temperature distributions in the zone of subduction of the Black Sea micro-plate under the Scythian plate with no effects of dissipative heating and convection taken into account for non-Newtonian rheology: (a, b) for the water content $C_w=10^{-3}$ weight %% and (c, d) for the water content $C_w=3\times10^{-1}$ weight %%. Parallel equidistant streamlines represent subducting Black Sea micro-plate, the streamlines above correspond to the mantle wedge flow induced by subduction.

Subducting plate was considered rigid, while the viscosity at the zone of plates friction (at temperatures below 1200 K) was reduced by 2 orders of magnitude as compared to (5). The latter viscosity reduction at the plates contact zone accounts for lubrication effected by deposits partially entrained by the subducting plate. Such a lubrication prevents the overriding Scythian plate from gluing to the subducting one [Gerya, 2011]. It is worth noting the isotherm $T=0.15$ in Fig.3a,c approximately corresponding to the Earth's surface is depressed at subduction zone by~7 km which is of the order of a typical trench depth. Fig.3 shows the results of computation for formulae (7) – (9) for non-Newtonian rheology case for the water content $C_w=10^{-3}$ weight %% (Fig.3a, b) and $C_w=3\times10^{-1}$ weight %% (Fig.3c, d). The velocity $V=45$ mm per year is chosen as resulting in the best convective zone size fitting in with the observed heat flux (positive and negative) anomaly size at the point C_2 in Fig.1, i.e. in the rear of the Mountainous Crimea. The Black Sea micro-plate subducting with a given velocity *V* is considered rigid and is shown in Fig.3b,d by the equidistant diagonal streamlines. The induced mantle wedge flow above the subducting plate is seen to occur in the form of a single vortex at $C_w=10^{-3}$ weight %% (Fig.3b) and in the form of the 2 vortices (located one above another) at $C_w=3\times10^{-1}$ weight %% (Fig.3d), the latter 2 vortices being considerably compressed in the vertical direction and the upper one (with $\psi > 0$) revolves clockwise while the lower one (with $\psi < 0$) revolves counterclockwise (Fig.3b,d). Micro-whirls 10^2 km great are formed between the counter-flows inside the upper induced flow obviously due to the tangential discontinuity instability (Kelvin-Helmholtz instability).

Assuming $Ra = 5.55\times10^8$ and $Di = 0.165$, i.e. switching dissipation and convection on, and taking into account the effects of phase transitions, from (1)–(2) the convection is found not to arouse in the non-Newtonian rheology case at $C_w=10^{-3}$ weight %%. At $C_w=3\times10^{-1}$ weight %% the 2 induced mantle flows in the mantle wedge are destroyed during the time interval ~0.6×10^{-6} (in dimensional form ~0.1 Myr) by the convective vortices shown in Fig.4 with the streamlines depicted with the interval of 4$\cdot$10^4.

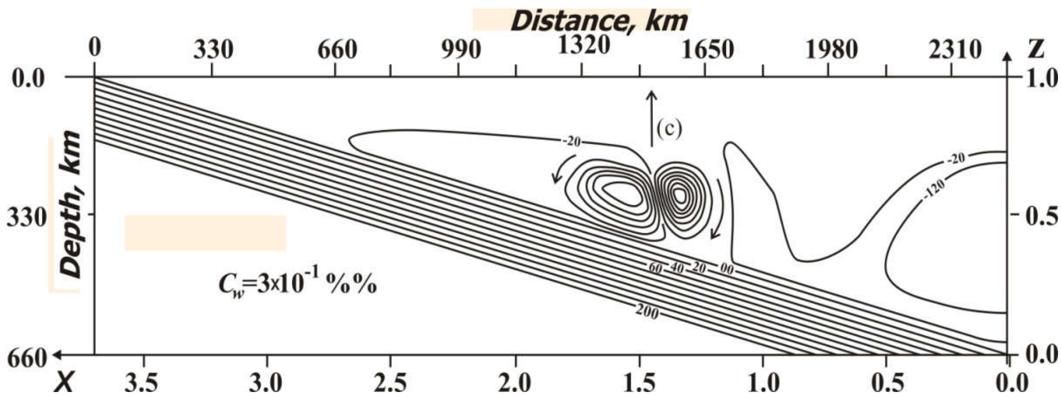

Fig. 4: Quasi steady-state stream-function in the mantle wedge with the effects of dissipative heating and convective instability for the case of non-Newtonian rheology and the water content $C_w=3\times10^{-1}$ weight %%. Arrow (c) shows ascending convective flow transporting mantle hydrocarbons to the Earth's surface at the point C_2 in Fig.1.

These convective vortices are seen actually to correspond to a single convection cell aroused at subduction velocity V=45 mm per year. The latter convection cell dimension is of the order of ~300 km, i.e., is very close to the observed minima *q* separation under the C_2 point in Fig.1.

Thus the for the non-Newtonian mantle wedge rheology case with the viscosity reduced by 3 orders of magnitude as compared to (7)– 9) the computation shows the convection in the mantle wedge to occur at $C_w=3\times10^{-1}$ weight %% in the form of two micro vortices at *V*=45 mm per year. Convection of this type can provide abnormal 2D heat flux *q* observed in the rear of the Mountainous Crimea and the upwelling of the mantle hydrocarbons to the Earth's surface along the arrow "c" [Yudin, 2003]. Considerable velocity in convective vortices in Fig.4 is due to the local viscous stresses increase resulting in the drop in viscosity in convective zone. In the case of Newtonian rheology the convection is aroused at the subduction velocity of over 10^2 mm$\times$a^{-1}, which appears unrealistic.

According to [Zharkov, 2019, p.143], the water content in the mantle transition zone in the mantle wedge may amount to ~3 wt. %. To investigate the role of water infused into the mantle wedge from the subducting slab the above computations were carried out for the mean water content of 1 wt. % and subduction velocity of 30, 20, and 10 mm per year. The results of the convection computation are shown in Figs.5a and 5b for *V*=30 and 20 mm per year respectively, where the streamlines corresponding to subducting Black Sea micro-plate are shown with the interval of 10, and the streamlines, corresponding to convective vortices with the interval of 10^6. The mean non-dimensional velocity in the left micro-vortex are ~15.2×10^7, ~7.1×10^7 and ~0.05×10^7 for the velocity of subduction of *V* = 30, 20, and 10 mm per year respectively. Thus, the convection may be considered to arise at the subduction velocity over ~10 mm per year for the mean water content C_w~1 wt.%. Since the meant water content in the mantle wedge could hardly exceed ~1 wt.% even at the water content in the mantle transition zone of 3 wt%, the obtained subduction velocity of ~10 mm per year may be regarded the minimum estimate of that of subduction of the Black Sea micro-plate.

It is worth noting, that in the case of Newtonian rheology, the mantle wedge dissipation-driven convection in the form of transversal rolls, as in Fig.4, is characteristic of very small subduction angles, the convection of this type being absent already at subduction angle β=30° [Gavrilov & Abbott, 1999]. At the subduction angle under consideration here, β=15°, the convective transversal rolls do not appear at $V<10$ cm×yr^{-1} for the Newtonian rheology case. Arrow (*c*) above the boundaries of the oppositely revolving convective vortices in Figs.4, 5 indicate a possible direction of transport of non-organic mantle hydrocarbons to the Earth's surface.

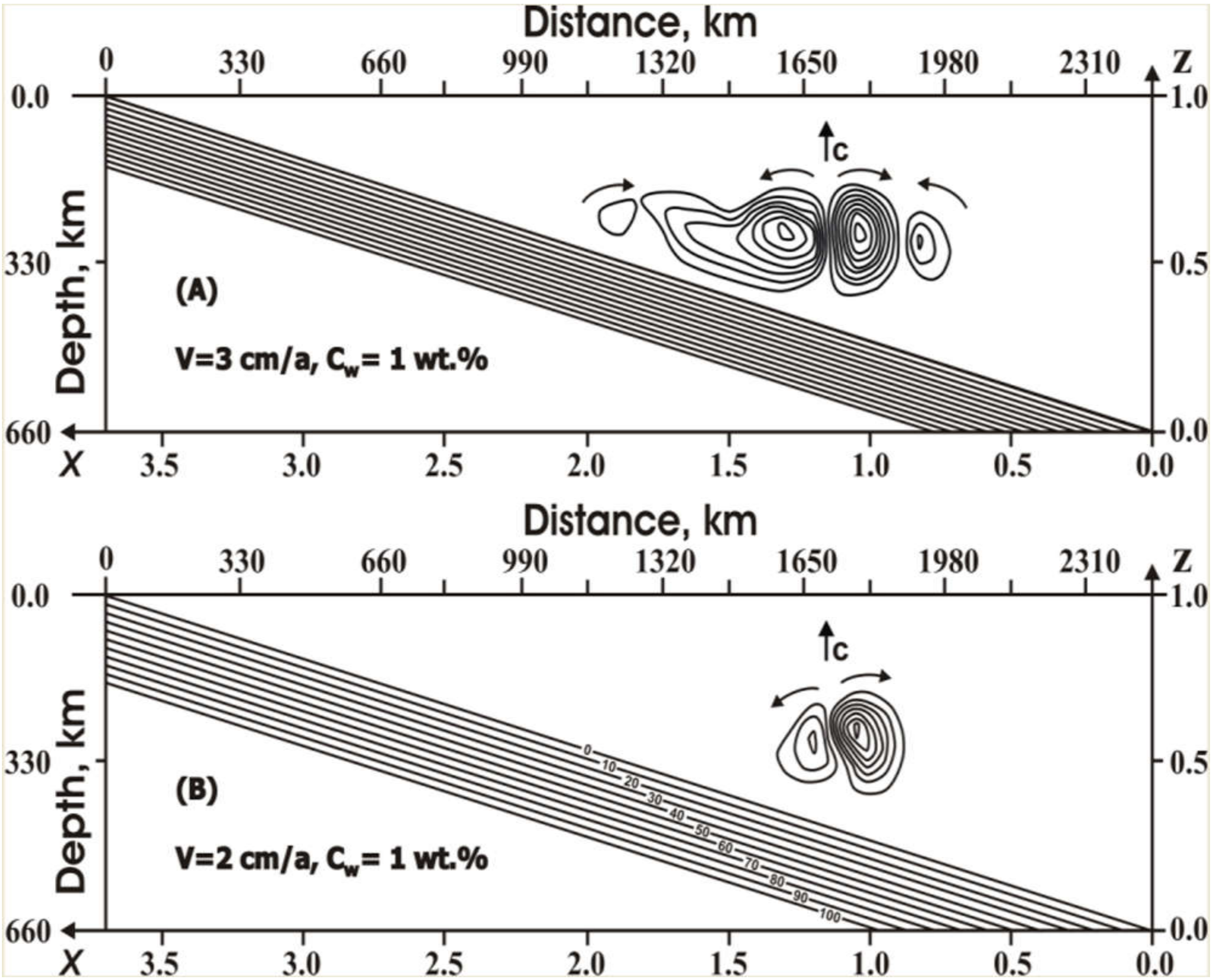

Fig. 5: Quasi steady-state stream-function in the mantle wedge with the effects of dissipative heating and convective instability for the case of non-Newtonian rheology and the water content C_w=1 wt. % at the subduction velocity of (a) – 30 mm per year and (b) – 20 mm per year. Arrow (*c*) shows ascending convective flow transporting mantle hydrocarbons to the Earth's surface at the point C_2 in Fig.1.

Computations for Newtonian mantle rheology with the viscosity (5)-(6) shows the transversal rolls to be aroused at far greater distance from the trench than the observed 2D heat flux anomaly. Thus the model constructed here favors the non-Newtonian mantle wedge rheology as better fitting in with the observed heat flux anomaly localization. It should be noted that numerous thermo-mechanical mantle models in the zones of subduction (see, e.g. [Gerya et al., 2006; Gerya, 2011] and the vast number of references there) showed convection in the form of transversal rolls never to occur as the models with extremely small subduction angle and sufficiently great subduction velocity were not investigated.

IV. Conclusions

The size of the cell of 2D mantle wedge dissipation-driven convection in the case of the realistic non-Newtonian rheology equals ~300 km at the subduction velocity 10 mm×yr^{-1} and the mean water content of ~1 wt.%, in which case a single convection cell is aroused. This explains the formation and horizontal extent (~250 km) of the only 2D heat flux anomaly observed in the rear of the Mountainous Crimea. The water content sufficient for the 2D convection to be aroused is ~1 wt. % at the velocity of a subduction of ~10 mm per year. The non-Newtonian model convection cell locates twice further from the trench than the observed 2D heat flux anomaly. The velocity in convective vortices in the non-Newtonian rheology case is ~10 m per year which may be sufficient to provide upward transport of mantle wedge hydrocarbons to the Earth's surface.

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