AGU PUBLICATIONS

Tectonics

Supporting Information for

Continental interior and edge breakup at convergent margins induced by subduction direction reversal: A numerical modeling study applied to the South China Sea margin

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Introduction

This supporting information provides governing equations, material parameters, and benchmarks used in the numerical experiments.

Supplementary material S1:

1.1 Governing equations

The mass conservation is described via the continuity equation with an incompressibility assumption:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_z}{\partial z} = 0 \qquad (1)$$

where v_x and v_z correspond to the horizontal and vertical components of the velocity vector, respectively.

The momentum conservation is approximated by 2D Stokes flow. The equation takes the form:

$$\frac{\partial \sigma'_{xx}}{\partial x} + \frac{\partial \sigma'_{xz}}{\partial z} = \frac{\partial P}{\partial x} \qquad (2)$$

$$\frac{\partial \sigma'_{zz}}{\partial z} + \frac{\partial \sigma'_{zx}}{\partial x} = \frac{\partial P}{\partial y} - g\rho(\mathrm{C, T, P}) \qquad (3)$$

where σ'_{xx}, σ'_{xz}, and σ'_{zz} are the deviatoric stress tensor components, g is gravitational acceleration, ρ is the density depending on the temperature (T), the pressure (P), and the composition (C).

The heat conservation equation is solved in a Lagrangian frame and takes the form:

$$\rho C_p \left(\frac{DT}{Dt}\right) = -\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} + H_r + H_a + H_S + H_L \qquad (4)$$

$$q_x = -k(T, P, C)\frac{\partial T}{\partial x} \qquad (5)$$

$$q_z = -k(T, P, C)\frac{\partial T}{\partial z} \qquad (6)$$

$$H_a = \mathrm{T}\alpha\frac{\mathrm{DP}}{\mathrm{Dt}} \qquad (7)$$

$$H_s = \sigma'_{xx}\dot{\varepsilon}_{xx} + \sigma'_{zz}\dot{\varepsilon}_{zz} + 2\sigma'_{xz}\dot{\varepsilon}_{xz} \qquad (8)$$

where x and z are the coordinates, DT/Dt is the substantive time derivative of temperature (T), the strain rate tensor is defined by $\dot{\varepsilon}_{xx}$, $\dot{\varepsilon}_{zz}$, $\dot{\varepsilon}_{xz}$, q_x and q_z are heat flux components, k *(T, P, C)* is the thermal conductivity as a function of temperature (T), pressure (P) and composition (C), C_p is the isobaric heat capacity, α is the thermal expansion coefficient. The equation considers the effect of radioactive (H_r), adiabatic (H_a), shear (H_S) and latent (H_L) heat production.

1.2 Rock rheology implementation

Visco-plastic-elastic rheology is adopted in this study, in which the rheological behavior is determined according to the minimum differential stress by comparing the viscous and plastic deformation. The viscous rheology behavior is computed based on the experimentally determined flow laws (*Ranalli, 1995*). The effective creep viscosity (η_{ductile})represents the competition between diffusion and dislocation creeps:

$$\eta_{ductile} = 1/(1/\eta_{diff} + 1/\eta_{disl}) \qquad (9)$$

Where η_{diff} and η_{disl} are given as:

$$\eta_{diff} = \frac{1}{2}A_d\sigma_{crit}^{1-n}exp\left(\frac{E_a+PV_a}{RT}\right) \qquad (10)$$

$$\eta_{disl} = \frac{1}{2}A_d\sigma_{II}^{1-n}exp\left(\frac{E_a+PV_a}{RT}\right) \qquad (11)$$

where σ_{II} is the second invariant of stress. A_d, E_a, V_a, and n are experimentally determined flow law parameters, which are material constant, activation energy, activation volume, and stress exponent, respectively.

$\sigma_{crit} = 10^4$ Pa is the stress that transfer from diffusion creep to dislocation creep (Turcotte and Schubert, 2002). Diffusion creep always exists in the model's deformation. When the yielding criteria is reached $\sigma_{II} >= \sigma_y$, plasticity dominants the deformation. Effective viscosity is constrained by the plastic yielding stress:

$$\eta_{effect} = \frac{\sigma_y}{2\dot{\varepsilon}_{\mathrm{II}}} = \frac{C_0 \cos(\arcsin(\phi)) + P_\phi}{2\dot{\varepsilon}_{\mathrm{II}}} \tag{12}$$

where σ_y is the plastic yielding stress; C_0 is the cohesion; ϕ is the coefficient of internal friction; and $\dot{\varepsilon}_{\mathrm{II}}$ is the second invariant of strain rate. At a situation with sufficient high stress and low temperature, Peierls creep takes over from dislocation creep. Constitution equation of Peierls creep can be expressed as below (Katayama and Karato, 2008):

$$\dot{\varepsilon}_{\mathrm{II}} = A_{Pei}\sigma_{\mathrm{II}}^2 exp\left\{-\frac{PV_a + E_a}{RT}\left[1 - \left(\frac{\sigma_{\mathrm{II}}}{\sigma_{Pei}}\right)^m\right]^n\right\} \tag{13}$$

where $\sigma_{Pei} = 9.1 \times 10^9$ Pa, $A_{Pei} = 6.3 \times 10^{-5}$ Pa^{-2}s^{-1}, experimentally determined parameters m and n are 1 and 2, respectively (Katayama and Karato, 2008).

The ductile rheology is combined with brittle to yield an effective visco-plastic, so the extended Drucker–Prager yield criterion is implemented as below (*e.g., Ranalli, 1995*):

$$\sigma_{yield} = C + Psin(\phi_{eff}) \tag{14}$$

$$sin(\phi_{eff}) = sin(\phi)(1 - \lambda) \tag{15}$$

$$\eta_{plastic} = \frac{\sigma_{yield}}{2\dot{\varepsilon}_{II}} \tag{16}$$

where σ_{yield} is the yield stress, $\dot{\varepsilon}_{II}$ is the second invariant of the strain rate tensor, P is the dynamic pressure, C is the cohesion, φ_{eff} is the internal friction angle, and λ is the pore fluid coefficient.

The equation of elasticity can be described as:

$$\dot{\varepsilon}_{ij(elastic)} = \frac{1}{2\mu}\frac{D\sigma_{ij}}{Dt} \tag{17}$$

Where μ is the shear modulus; $D\sigma_{ij}/Dt$ is the objective co-rotational time derivative of the deviatoric stress components σ_{ij}.

1.3 Partial melting model

Modeling accounts for the partial melting using experimentally determined wet solidus and dry liquidus curves in the pressure-temperature domain. As a first approximation, the melt fraction (M) is assumed to increase linearly with T based on the following expression (*Gerya and Yuan, 2003; Burg and Gerya, 2005*):

$$M = 0, at\ T \leq T_{solidus} \tag{18}$$

$$M = \frac{(T - T_{solidus})}{(T_{liquidus} - T_{solidus})}, at\ T_{solidus} < T < T_{liquidus} \tag{19}$$

$$M = 1, at\ T \geq T_{liquidus} \tag{20}$$

where $T_{solidus}$ and $T_{liquidus}$ are the solidus and liquidus temperature of the given lithology, respectively. The effective density (ρ_{eff}) of molten rocks varies with the M, P, and T according to the following expression:

$$\rho_{eff} = \rho_{solidus} \left(1 - M + M \frac{\rho_{molten}}{\rho_{solidus}}\right) \quad (21)$$

where $\rho_{solidus}$ and ρ_{molten} are the densities of the solidus and molten solid rock, respectively. The $\rho_{solidus}$ and ρ_{molten} are computed at a given P and T based on the following equation:

$$\rho_{P,T} = \rho_0 \left[1 - \alpha(T - T_0)\right]\left[1 + \beta(P - P_0)\right] \quad (22)$$

where ρ_0 is the density of the dry mantle at reference P_0 of 0.1 MPa and T_0 of 298 K; α and β are the thermal expansion and compressibility coefficients, respectively.

The effect of latent heating H_L is computed by an increased effective heat capacity (C_{Peff}) and the thermal expansion (α_{eff}) of the partially molten solid rock ($0 < M < 1$) according to the following relations:

$$C_{Peff} = C_P + Q_L \left(\frac{\partial M}{\partial T}\right)_P \quad (23)$$

$$\alpha_{eff} = \alpha + \rho \frac{Q_L}{T} \left(\frac{\partial M}{\partial T}\right)_T \quad (24)$$

where α and C_P are the thermal expansion and heat capacity, respectively. Q_L is the latent heat of melting of the solid rock.

1.4 Topographic model

A weak stick air ($\eta=10^{18}$ Pa·s, $\rho=1$ kg/m^3) or water layer ($\eta=10^{18}$ Pa·s, $\rho=1000$ kg/m^3) is applied on the upper surface to provide a free-surface-like condition that allows topographic evolution (*Crameri et al., 2012*). The interface between weak stick air/water layer and the underlying crust can be viewed as an internal erosion/sedimentation surface. The erosion and sedimentation processes are developed by solving the transport equation in Eulerian coordinates at each time step (*Gerya and Yuen, 2003*).

$$\frac{\partial z_{es}}{\partial t} = v_z - v_x \frac{\partial z_{es}}{\partial x} - v_s + v_e \quad (25)$$

where z_{es} is the vertical position of the surface, v_x and v_z are the vertical and horizontal components of the material velocities, respectively. v_e and v_s are the erosion and sedimentation rates, respectively. We use a moderate erosion/sedimentation rate of 0.3 mm/yr in this study.

Table S1: Material parameters used in the numerical experiments. See the text for the explanations of the symbols. Other properties (for all rock types): C_P=1000 J kg^{-1}K^{-1}, α=3×10−5 K^{-1}, β =1×10^{-11} Pa^{-1}. References: 1 Turcotte and Schubert, 2002; 2 Bittner and Schmeling, 1995; 3 Clauser and Huenges, 1995; 4 Schmidt and Poli, 1998; 5 Hess, 1989; 6 Hirschmann, 2000; 7 Johannes, 1985; 8 Poli and Schmidt, 2001; 9 Hofmeister 1999; 10 Turcotte and Schubert, 1982; 11 Ranalli, 1995 and references therein.

Material	ρ_0, kg/m^3	sin(φ_{eff})	AD, MPa^{-n}s^{-1}	n	V, J/(MPa·mol)	E, kJ/mol	H_r, μW/m^3	$T_{solidus}$, K	$T_{liquidus}$, K	k, W/(m K)
Sediments (wet quartzite)	2700	0.03	3.2e-4	2.3	0	154	2	889+17900/(P+54)+ 20200/(P + 54)^2 at P < 1200MPa; 831+0.06P at P>1200 MPa	1262 + 0.09P	[0.64+807/(T+77)]* exp(0.00004P_{MPa})
Upper continental crust	2800	0.2					1			
Upper oceanic crust	3200	0.03					0.25			
Lower oceanic crust (plagioclase An_{75})	3200	0.2	3.3e-4	3.2	0	238	0.25	973-70400/(P+354)+ 77800000/(P+354)^2 at P<1600 MPa,935+ 0.0035P+0.0000062P^2 at P > 1600 MPa	1423 + 0.105P	[1.18+474/(T+77)]* exp(0.00004P_{MPa})
Lower continental crust	2900									
Lithospheric mantle (dry olivine)	3300	0.6	2.5e+4	3.5	10	532	0.022	1394+0.132899P- 0.000005104P^2 at P<10000 MPa 2212 + 0.030819 (P –10000) at P > 10000 MPa	2073 + 0.114P	[0.73+1293/(T+77)] *exp(0.00004P_{MPa})
Asthenospheric mantle										
Hydrated mantle (wet olivine)	3300	0.03	2.0e+3	4.0	10	471	0.022	1240+49800/(P+323)at P<2400MPa,1266- 0.0118P+0.0000035P^{2}a t P>2400 MPa	2073 + 0.114P	[0.73+1293/(T+77)] *exp(0.00004P_{MPa})
References	1,2	11	11	11	10,11	11	1,2 1	4,5,6,7,8	4	3,9

Supplementary material S2:

The simulations in this study are performed using the example "viscoelastic-plastic subduction" out of Taras Gerya's book, which is a 2-D thermomechanical code solving the Stokes and heat transfer equations (Gerya, 2010). The computer code used to generate our 2-D thermomechanical numerical model is provided in Gerya (2010), which is available online at www.cambridge.org/gerya.

In order to test the code's robustness, the book has conducted several benchmarks to verified the efficacy of numerical solutions. Please see **Chapter 16** for details of benchmarks in a variety of circumstances relevant to geodynamics (Gerya, 2010).

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