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Supplements to: The role of surface processes in basin inversion and breakup unconformity

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Contents:

SUPPLEMENTAL METHODS

We solve the problem of conservation of mass, momentum and energy for incompressible mantle flow and lithosphere deformation, using *Underworld2* - an open source particle-in-cell finite-element code (freely available at underworldcode.org) - in conjunction with the *UWGeodynamics* library, an open-source python library for more user-friendly interaction with *Underworld2*. The input files used in this work can be found here: https://github.com/LukeMondy/Continental_Rifting

We assume a visco-plastic rheology depending on temperature, stress, strain, strain rate, and in some experiments melt fraction (see Table S1). The densities of all rocks depend on temperature (see Table S1).

Experimental setup

The experiments are run within a Cartesian box of 600 km (x-axis) by 220 km (y-axis), which is defined from -300 km to 300 km (x), and -200 km to 20 km (y). The computational grid dimensions for solving the visco-plastic Stokes problem is 608×224 (~1 km cells). A 10 km wide and 2 km deep rectangle of lower crust is defined at the top of the lithospheric mantle (centred around x = 0 km), to preferentially localise deformation in the centre of the domain (Van Wijk and Blackman, 2005). An initial random plastic strain (up to 5%) is imposed the crust to model existing damage and faulting.

Fundamental equations

Underworld solves the incompressible equations of continuity for momentum, energy, and mass as below:

$$\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} = -\rho g \lambda_i$$

$$\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\kappa \frac{\partial T}{\partial x_i}\right) + Q$$

$$\frac{\partial u_i}{\partial x_i} = 0$$

Where x_i are the spatial coordinates, u_i is the velocity, T is temperature, ρ is density, g is gravity, λ_i is the unit vector in the direction of gravity, t is time, κ is thermal diffusivity, and Q is a source term for the energy equation. Summation on repeated indices is assumed.

Additional terms can be incorporated into the above equations. In the experiments presented, only radiogenic heating is added, unless explicitly mentioned otherwise - however, an additional experiment was run with partial melting, and so the associated terms and values are described below.

Both radiogenic heating and the thermal aspects of partial melting are incorporated into the energy equations as:

$$Q_{\mathrm{radiogenic}} = \frac{A}{\rho C_p}$$

$$Q_{\text{partial melt}} = -1 \times \frac{L_f}{C_p}\frac{\delta M_f}{\delta t}$$

Where A is the rate of radiogenic heat production, C_p is heat capacity, L_f is latent heat of fusion, and M_f is the melt fraction.

The density of a material is defined via a function that depends on temperature and the melt fraction:

$$\rho = \rho_r \times (1 - \alpha(T - T_r) - (M_f \times M_{\Delta\rho_r}))$$

Where ρ_r is reference density, α is thermal expansivity, T_r is reference temperature, and $M_{\Delta\rho_r}$ is the fraction of density change when melted.

The melt fraction is calculated dynamically as part of the experiment, by using the super-solidus formula given by McKenzie and Bickle (1988):

$$SS = \frac{(T - T_s)}{(T_l - T_s)} - 0.5$$

$$M_f = 0.5 + SS + (SS^2 - 0.25) \times (0.4256 + 2.988 \times SS)$$

Where SS is the normalised super-solidus temperature, T_s is the solidus, and T_l is the liquidus.

The solidus and liquidus are defined as:

$$T_s = t_1 + t_2 P + t_3 P^2$$

Where P is pressure, t_1, t_2, and t_3 are defined Table S1.

The constitutive behaviour is assumed to be visco-plastic rheologies. For the viscous component, flow is computed using dislocation creep (Hirth and Kohlstedt, 2003):

$$\dot{\varepsilon}_{\text{disc}} = A\sigma^n d^{-p} f_{H_2O}^r \exp\left(-\frac{E + PV}{nRT}\right)$$

Where $\dot{\varepsilon}$ is the effective strain-rate, A is the pre-exponential factor, n is the stress exponent, d is the grain-size, p is the grain-size exponent, f_{H2O} is the water fugacity, r is the water fugacity exponent, E is the activation energy, P is the pressure, V is the activation volume, R is the gas constant, and T is the temperature.

For the plastic component, failure is determined using the Drucker-Prager model:

$$\sqrt{J_2} = Ap + B$$

Where $\sqrt{J_2}$ is the second invariant of the deviatoric stress tensor, p is the pressure, and A and B are defined as:

$$A = \frac{2sin\phi}{\sqrt{3}(3 - sin\phi)}$$

$$B = \frac{6Ccos\phi}{\sqrt{3}(3 - sin\phi)}$$

Where C is the cohesion, and ϕ is the friction coefficient.

A linear strain-softening function is applied to the plastic component. As strain is accumulated from 0 to 20%, the material linearly weakens from its original cohesion and friction coefficient to their softened equivalents (defined in see Table S1). Once fully weakened, the cohesion and friction coefficient remain constant at the softened values.

A stress limiter is applied to all rheologies, to limit the total strength of the lithosphere. The stress limiter is based on the work flow from Watremez et al. (2013), where a Von Mises criterion is applied, where:

$$\sqrt{J_2} = C$$

All materials are limited to 300 MPa in strength via this method, to account from pseudo-plastic processes, such as Peierls creep, and to ensure the lithosphere does not become artificially strong (Demouchy et. al., 2013; Zhong and Watts, 2013). To ensure numerical stability, all rock materials also have a minimum and maximum viscosity range of 1e19 Pa.s to 5e23 Pa.s.

Partial melting has a mechanical effect, whereby material undergoing melt will reduce in viscosity, within a given melt fraction range (defined in Table S1), based on the following model:

$$\eta_{melted} = \eta \times (1 \times M_{f\%} + \eta_{factor} \times (1 - M_{f\%})$$

Where η_{melted} is the viscosity after melting, η is the viscosity calculated from the flow law, $M_{f\%}$ is a normalised linear interpolation of the melt fraction between the lower and upper limits of the melt fraction range, and η_{factor} is the melt viscous softening factor the material undergoes once fully melted.

Rheologies

The rheologies used are based on published work: the upper crust flow law is a wet quartzite from Paterson and Luan (1990); the lower crust flow law is a mafic granulite from Wang et. al (2012); and the lithospheric mantle flow law is a wet olivine from Hirth and Kohlstedt (2003). Viscous flow laws that use 0 for the water fugacity exponent typically have this effect incorporated into the pre-exponential factor. Radiogenic heat production values are from Hasterok and Chapman (2011). Melt and other parameters derived from Rey and Müller, (2010). The air material uses an isoviscous 1e18 Pa.s flow law, with a density of 1 kg m^{-3}, thermal expansivity of 0 K^{-1}, and a heat capacity of 1000 J K^{-1}. See Table S1 for detailed parameters values.

Boundary conditions

Isostatic bottom

A constant pressure boundary condition is defined along the bottom wall to model isostatic equilibrium. The pressure applied is calculated at the beginning of the experiments by calculating the lithostatic pressure across the entire domain, and using the average pressure from along the bottom wall. This value is then applied throughout the entire experiment.

Using a constant pressure boundary condition on the base of the model removes a significant constraint on the vertical position of the material in the domain, which can lead to instabilities and large artificial vertical velocities. To help stabilise the experiments, the vertical walls use a no-slip velocity boundary condition, and the top wall has a free-slip, no flux boundary condition (that is, no material can pass through the top wall).

Free surface and top wall boundary condition

To emulate a free surface, the experiments all use an air layer. The air material cannot be modelled at natural values of viscosity or thermal expansivity, since it would be numerically very expensive and unstable. A common substitute is to use a "sticky-air" layer, which has unrealistically high viscosity, but is low enough to not interfere with underlying geodynamics. The isostatic criterion formula from Crameri et. al, 2012 (*eq* 12) gives a criterion for determining the thickness and viscosity of a good sticky-air layer. Based on this, our experiments use an air-layer with a viscosity of 1e18 Pa.s, and a thickness of 20 km.

The top wall has a free-slip, no flux boundary condition. The no flux condition helps stabilise the isostatic boundary condition on the wall, since it fixes the vertical position of the material in the domain. However, it also means that air material cannot flow in or out of the domain as topographic highs and lows form. Therefore, we give the air a high compressibility, so that it can expand or contract as required.

Thermal boundary conditions

The top wall of the model domain is held constant at 293.15 K (20°C) along with any air material, and the bottom wall is held at 1623.15 K (1350°C). Before the experiment is run, the asthenosphere has an additional boundary condition, so that it too is held at 1623.15 K (1350°C). The model is then thermally equilibrated to achieve a steady state geotherm. Once the experiment start, the asthenospheric boundary condition is removed. Throughout the experiments the temperature of the air layer is maintained at 20ºC, while the temperature in the asthenosphere, from 140 km to the base of the model, is maintained at 1350ºC.

Surface processes

Sedimentation and erosion are computed by a simple elevation threshold calculation. Air particles that reach a certain elevation are converted into sediment material, and any rock material particles that certain elevation are converted into air material. This process occurs at the end of each timestep. Surface processes cease when a 'gap' condition is met. At the beginning of the experiment, a line of passive tracer particles are distributed along the moho at 2 km spacing. As the experiment evolves, the largest gap between particles is evaluated, and if it exceeds the 'gap' parameter set (in our experiments, either: 30 km, 60 km, 80 km, or 100 km), then any surface processes are stopped. Functionally this results in the biggest gap being between the two margins that form, as the upwelling asthenosphere splits both the crust and the line of passive tracers.

This method of surface processes is both not physically accurate, and does not conserve mass. However, we believe this method is sufficient our experiments, since: a) the details of the process of basin formation is not necessarily the focus of this work, and b) the experiments are in a 2D setting. Since surface processes are fundamentally a three dimensional process, any mass-balancing methods of surface processes used in 2D would be similarly artificial.

Numerical parameters

Time stepping

Time stepping in Underworld uses the Courant-Friedrichs-Lewy (CFL) condition to ensure stable convergence. The CFL is a function of grid size, absolute maximum velocity, and maximum diffusivity. On top of this, to ensure a numerically efficient and temporally stable model run, the computed CFL timestep is multiplied by a factor of 0.1.

Solver parameters

The isostatic boundary condition used in these experiments is particularly sensitive to both the timestep size, and the solver parameters used. Underworld2 provides a tool called the penalty method, which is effective in solving difficult nonlinear problems - however, it is not compatible with compressible materials. Instead, we use stricter tolerances on the direct solver, with the nonlinear tolerance at 5e-4, and the linear solver tolerance at 1e-8. These parameters (along with the reduced CFL factor) produce very stable experiments, with very little velocity jumps and the associated strain-rate ‘oscillating’.

SUPPLEMENTAL FIGURES

Figures S1-S3 show the evolution of different aspects of all experiments. In each figure, the columns represent a single experiment with a particular imposed extension velocity. Each row represents a 5% increase in the applied kinematic extension, starting from 5%, and increasing until the experiment finishes. Each set of experiments is grouped by the gap distance, which is defined as how large the distance between the two rifted margins can get before surface processes are turned off.

Figure S1: Mechanical evolution of all experiments. Colours are the same as defined in Figure 2 from the main text.

Figure S2: Tectonic regime evolution of all experiments. Blue colours show regions in extension, red colours show regions in compression. Solid colours are where the plunge of the relevant principal stress is 90 degrees (vertical), which fades to white as the plunge reaches 60 degrees. Areas in white have no defined Andersonian stress.

Figure S3: Tectonic regime mediated by deviatoric stress evolution of all experiments. Colours are defined in the same way as Figure 3 from the main text.

Figure S4: Statistics of basement depth through all experiments. Colours and symbols are the same as described in Figure 4 of the main text.

Figure S5: The **Left panel** displays a simplified model of a rifted margin in isostatic equilibrium, showing three columns A, B and C. Lithospheric column **A** is the non-deformed lithosphere, it has a thickness of 140 km, including a crust 40 km in thickness. The lithospheric column **B** has crust and lithospheric thickness halved, while column **C** represents the situation at the Mid Oceanic Ridge (MOR). The density of the crust is 2700 kg.m^{-3}, that of the lithospheric mantle is 3330 kg.m^{-3}, and the density of the asthenosphere is 3300 kg.m^{-3} taking into account thermal expansion. The top of Column A, B and C stands at 0 km, 3.182 km, and 6.363 km depth respectively. Disregarding the weight of water, the **Right panel** shows the pressure difference profile between each column. In panel A the green profile shows the pressure difference between column A to column B, and a blue profile shows the pressure difference between column A to column C. The grey area shows the summation of the pressure differences. Panel B shows that column B experiences a complex depth-dependent differential stress pattern involving regions in extension and regions in compression, as the pressure difference derives from both column A and C.

Table S1

Parameter	Sediment	Upper Crust	Lower Crust	Mantle/Astheno
Reference density, ρ_r(kg m^{-3}) at 293.15 K	2600	2700	2900	3370
Thermal expansivity, α (K^{-1})	3e-5			
Heat capacity, C_p(J K^{-1} kg^{-1})	1000			
Thermal diffusivity, α(m^2 s^{-1})	1e-6			
Latent heat of fusion, L_f(kJ kg^{-1})	250			450
Radiogenic heat production, A (W m^{-3})	1.2e-6		0.6e-6	0.02e-6
Melt density change fraction, $M_{\Delta\rho_r}$	0			
Liquidus term 1, t_1 (K)	1493			2013
Liquidus term 2, t_2 (K Pa^{-1})	-1.2e-7			6.15e-8
Liquidus term 3, t_3 (K Pa^{-2})	1.6e-16			3.12e-18
Solidus term 1, t_1 (K)	993			1393.661
Solidus term 2, t_2 (K Pa^{-1})	-1.2e-7			1.32899e-7
Solidus term 3, t_3 (K Pa^{-2})	1.2e-16			-5.104e-18
Friction coefficient	0.55		0.577	0.577
Softened friction coefficient	0.055		0.2308	0.02308
Cohesion, C (MPa)	10		20	10
Softened cohesion, C (MPa)	2		0.8	0.4
Pre-exponential factor, A (MPa^{-n} s^{-1})	6.60693e-8		10e-2	1600
Stress exponent, n	3.1		3.2	3.5
Activation energy, E (kJ mol^{-1})	135		244	520
Activation volume, V (m^3 mol^{-1})	0		0	23e-6
Water fugacity	0		0	1000
Water fugacity exponent	0		0	1.2
Melt viscous softening factor	1e-3		1e-3	1e-1
Melt fraction range for viscous softening	0.15 - 0.3		0.15 - 0.3	0 - 0.02

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