

Supplementary

COMSOL test for thermo-chemical mantle convection

COMSOL Multiphysics v4.2a finite element numerical model package was used to simulate thermo-chemical convection occurring in the Earth's mantle. In order to estimate the accuracy and limitation of the method and the model results two comparison tests were carried out. A benchmark paper by van Keken et al. (1997) was used to qualify the solution.

Test 1 is an isothermal Rayleigh–Taylor problem in which a light layer with a thickness of 0.2 is situated at the bottom of the 2D model domain with an aspect ratio 1×0.9142 . Boussinesq approximation of the equations governing the thermo-chemical convection was applied. The two non-dimensional parameters, the thermal and the compositionally Rayleigh number were $Ra=0$ and $Rb=1$, respectively. The comparison was made based on four quantities: the growth rate of the instability obtained from rms velocity, γ ; the maximum rms velocity of the system, v_{max} ; the time at the maximum velocity, t_{max} ; and time variation of the entrainment rate, $e(t)$. For details see paper of van Keken et al. (1997). The maximum element size (similarly to resolution applied in the companion paper) was 0.017 in the model domain decreasing to 0.01 and 0.005 toward the boundaries closing round the upper dense and the lower light layer, resp.

In the test the light lower layer becomes unstable and a plume evolves on the left of the model domain (*Figure S1.b*). A secondary plume with less buoyancy forms on the right side of the box to entrain the remnant of the light material upward (*Fig. S1.c*). Compositionally dense plumes break through the forming upper light layer to transport the nearsurface remnant of the dense material downward (*Fig. S1.d*). Snapshots of the concentration field are in accordance with the solutions of marker chain, field and tracer methods presented in the benchmark paper. Results from COMSOL seem to be qualitatively better than the SK field method but with smeared transition in the concentration related to the other methods.

Figure S2 shows the root mean square velocity and the entrainment rate as a function of non-dimensional time. The ascension of the first plume with large buoyancy forms the global maximum in velocity, then the secondary plume on the right side of the box produces the local maximum later. The two intense phase facilitates the mixing resulting in a steep increase of the entrainment. The velocity and the entrainment time series are located among the tracer and marker chain methods. As concerns the quantities, the growth rate of the instability is $\gamma=0.001136$, the maximum velocity is $v_{max}=0.003085$ and the time at the maximum velocity is $t_{max}=208.53$. These data agree very well with the results from tracer methods and are a bit further from the results of marker chain and field methods.

Test 2 was accomplished to investigate the mixing of the dense material by thermal convection. The compositionally dense layer with a thickness of 0.025 was positioned at the bottom of the model box with an aspect ratio of 1×2 . The non-dimensional numbers characterizing the thermo-chemical system in Boussinesq approximation were $Ra=3 \cdot 10^5$ and $Rb=4.5 \cdot 10^5$ (buoyancy ratio is $B=Rb/Ra=1.5$), and the Lewis number which is the ratio of the thermal and chemical diffusivity was $Le=10^{14}$ during the simulation. The velocity and the entrainment time series as well as five snapshots of the composition field were used to qualify the method. The entrainment was calculated for the domain between 0.2 and the surface. Because the dense layer was thin higher resolution was applied, the maximum element size was 0.0051 and 0.0017 above and below the depth of 0.2, respectively.

Figure S3 displays the evolution of the compositionally dense layer. At time of $t=0.01$ the concentration distribution qualitatively agrees well with the solutions from the other methods. From $t=0.015$ results becomes diverging, at $t=0.02$ – 0.04 our solution is comparable to the HS tracer and SK field methods. At the end of the model run ($t=0.05$) COMSOL

produces more intense mixing than other methods and results in only a small part of the dense material in the lower domain. *Figure S4* illustrates the velocity and the entrainment rate time series. Velocity agrees with the results from other methods to $t=0.015$, from where the solutions start diverging from each other. The entrainment rate confirms the conclusions from concentration snapshots, i.e. $e(t)$ is comparable to HS tracer and SK field methods to $t=0.4$, then the entrainment accelerates related to the other methods.

References

Van Keken, P. E., King, S. D., Schmeling, H., Christensen, U. R., Neumeister, D., and Doin, M.-P.: A comparison of methods for the modeling of thermochemical convection, *J. Geophys. Res.*, 102, 22477–22495, 1997.

Figure captions

Figure S1

Snapshots of the concentration field during the Rayleigh-Taylor instability test.

Figure S2

Root mean square velocity and entrainment rate time series during the Rayleigh-Taylor instability test.

Figure S3

Snapshots of the concentration field during the thermo-chemical instability test.

Figure S4

Root mean square velocity and entrainment rate time series during the thermo-chemical instability test.