Today it is possible to model thermal-chemical convection and mantle dynamics taking into account thermodynamics and rheological properties of multi-phase aggregates. First principles calculations are nowadays offering input for these simulations that cannot be obtained by other means. Particularly important is the knowledge of phase boundaries and changes in properties resulting from phase transitions. Contrast in properties across the post-perovskite transition in the deep mantle computed by first principles by Tsuchiya et al., were used to perform novel simulations. This transition appears to inhibit the formation of superplumes unless some form of radiative heat transport is included in these simulations.


Comparison between two-dimensional upwelling developments for constant thermal conductivity (top panel) and for radiative thermal conductivity (bottom panel) in thermal-chemical convection including both, the post-spinel transition in the transition zone, and the post-perovskite transition above the core mantle boundary.

http://vlab.msi.umn.edu

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Thermal-Chemical Convection Simulations Including Materials Properties Obtained by First Principles

Temperatures with PPP for weaker temperature dependence of viscosity (two orders of magnitude)