Numerical and laboratory studies of mantle convection: Philosophy, accomplishments and thermo-chemical structure and evolution

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Since the acceptance of the theory of plate tectonics in the late 1960s, numerical and laboratory studies of mantle convection and plate tectonics have emerged as a powerful tool for understanding how the solid parts of Earth and other terrestrial planets work. Here, the general philosophy of such modeling is discussed, including what can and cannot be determined, followed by a review of some of the major accomplishments and findings. Then some recent work by the authors on thermochemical convection is reviewed, with a focus on comparing the results of numerical experiments to observations from geochemistry, seismology and geomagnetism in order to constrain uncertain physical parameters. Finally, the future of such research is discussed.

1. Modeling Philosophy and Accomplishments

Geodynamic theory plays a central role in understanding the solid Earth, as it provides a bridge or framework that links together the various other subfields, particularly seismology, mineral physics, geochemistry, geodesy, and geology. The foundation of this framework is the theory of continuum mechanics, which provides a quantitative theory linking forces within the Earth to subsequent displacements. Mineral physics plays a crucial role in geodynamic theory by providing the constitutive relations that link relevant intensive (e.g. stress, temperature, chemical potential, etc.) and extensive (e.g. strain, entropy, composition, etc.) variables. Mineral physics provides the physical properties (e.g. rheology, equation of state, heat capacity, thermal conductivity, etc.) necessary for a forward calculation of convection and plate tectonics, which can then predict the nature of seismic wave velocity anomalies, geochemical heterogeneity and geodetic observations (velocities, gravitational field) for comparison to observations. Alternatively, wave speed anomalies detected by seismology can be converted to buoyancy anomalies using mineral physics, then geodynamic theory can be used to compute surface gravitational anomalies, topography and velocities.

It is useful to recognize the fundamental difference between what is obtained by observation-based fields such as geochemistry and seismology, and geodynamic theory. While observations, leading for example to seismic tomographic models, are giving us an increasingly resolved picture of the structures present inside the mantle, seismic tomography is merely a mathematical fit to the observations-describing *what* is there, analogous to Kepler's laws which give a mathematical fit to the orbits of planets round the Sun. Geodynamics, however, goes beyond this and provides the fundamental explanation of *why* these structures occur, which is analogous to Newton's laws explaining why planets move round the Sun as they do. Thus, even if seismological observations could map out three-dimensional Earth structure to a resolution of 1 km, dynamical modeling would still be necessary in order to understand why the observed structures occur.

In addition to explaining observations, convection investigations also offer a predictive capability, i.e., predicting what is expected to be found once observational techniques improve enough to observe them. Two prominent examples of this are: (i) Based on numerical experiments of convection plus consideration of geoid and surface topography (e.g., [*Davies*, 1988]), the geodynamics community was strongly in favor of predominantly whole-mantle convection, perhaps with slabs intermittently held up above the 660 km discontinuity [*Christensen and Yuen*, 1984; *Christensen and Yuen*, 1985; *Machetel and Weber*, 1991; *Peltier and Solheim*, 1992; *Tackley*, 1995], long before seismology gave us conclusive images that supported this view [*Van der Hilst et al.*, 1997]. (ii) Laboratory and numerical experiments predicted the existence and dynamics of upwelling plumes (e.g., [*Griffiths and Campbell*, 1991; *Morgan*, 1971; *Olson and Singer*, 1985; *Whitehead and Luther*, 1975]) long before seismology became capable of imaging them in the deep mantle [*Montelli et al.*, 2004]. Of course, this predictive capability is limited by uncertainties in physical parameters and model simplifications as discussed later.

Several distinctions can be made regarding different types of study. One distinction is between studies that investigate the basic fluid dynamics to understand scalings, regimes of behavior, phenomenology etc., and studies that attempt to match specific observations, be it seismological, geochemical, geological, or geodetic. As the field progresses, there has been a progression from more emphasis on the former, to more emphasis on the latter. Another distinction regards the timescale that is being modeled, which ranges from instantaneous (e.g., studies that attempt to match the geoid using flow calculated from seismic tomography), to short-term (e.g., the last 120 Ma of Earth history), to long-term- either 'evolution' scenarios that represent the inherently transient evolution of Earth or another planet over 4.5 billion years, or experiments that produce a 'statistically steady-state'. The level to which specific observations can be matched increases as timescale is decreased, mainly because the short term or instantaneous experiments require imposing the model setup or initial conditions such that observations are matched. Each of these approaches has its place, depending on the questions being posed; ultimately all are necessary. For example a physical description of the mantle that is able to match some instantaneous or recent geological observation on Earth is clearly not perfect if when run for billions of years it produces a planet that looks nothing like Earth, and the reverse also applies.

Both laboratory and numerical approaches have been used, with numerical approaches becoming more prevalent as computational technology has improved. Numerical calculations are best thought of as 'experiments' in the same sense as laboratory experiments, rather than 'simulations', as the latter implies an attempt to simulate the real Earth, which is still some distance from what is numerically possible. Experimental studies, whether laboratory or computational, should have a clearly defined setup, including approximations made and the extent to which results are applicable to real planets, and well posed questions to be answered.

Many fundamental concepts, scalings and phenomena have been established by experiments and theory, Several examples, a few of which (certainly not all) have become so engrained in our collective consciousness such that they are taken for granted, are given below.

(i) The onset of convection in terms of Rayleigh number [*Chandrasekhar*, 1961; *Holmes*, 1931] including heating from within [*Roberts*, 1967], and the planforms of convection that appear as Rayleigh number is increased (e.g., [*Schubert and Zebib*, 1980; *Zebib et al.*, 1983; *Zebib et al.*, 1980]).

(ii) The basic structure of a convection cell, with narrow boundary layers thickening approximately as a half-space solution and near-adiabatic interior (e.g., summarized in [*Turcotte and Schubert*, 1982]).

(iii) The scaling of heat flux and velocity with Rayleigh number for constant-viscosity convection as predicted by boundary layer theory and verified by numerical experiments (e.g., [*Jarvis and Peltier*, 1982; *Turcotte and Schubert*, 1982]).

(iv) The concept of plumes and their structure and dynamics (e.g., [*Campbell and Griffiths*, 1990; *Morgan*, 1971; *Olson and Singer*, 1985; *Parmentier et al.*, 1975]).

(v) The influence of temperature-dependent viscosity, including the transition to rigid lid convection at high viscosity contrast [*Christensen*, 1984b; *Moresi and Solomatov*, 1995; *Nataf and Richter*, 1982; *Ogawa et al.*, 1991; *Ratcliff et al.*, 1997; *Solomatov*, 1995] and its influence on thermal evolution [*Tozer*, 1972].

(vi) The basic planform of three-dimensional convection, with ridge-like boundary layer instabilities that become more plume-like as they cross the domain, and the influence of internal heating- raising the internal temperature, making the downwellings more plume-like and the interior sub-adiabatic, (e.g., [*Bercovici et al.*, 1989; *Houseman*, 1988; *Parmentier et al.*, 1994; *Travis et al.*, 1990])

(vii) The influence of non-Newtonian rheology, localizing deformation and making the system much more episodic, (e.g., [*Christensen*, 1983; *Christensen and Yuen*, 1989; *Parmentier et al.*, 1976]).

(viii) The influence of depth-dependent viscosity and thermal expansivity in making deep mantle upwellings broader and increasing the horizontal wavelength of flow (e.g., [*Balachandar et al.*, 1992; *Hansen et al.*, 1993; *Tackley*, 1996]).

(ix) The realization that plate tectonics itself is a particular manifestation of more general behavior arising from mantle processes/convection in terrestrial planets, and is unique to planet Earth at the present time.

(x) The ability of plastic yielding to break a rigid lid and generate a crude approximation of plate tectonics (e.g., [*Moresi and Solomatov*, 1998; *Tackley*, 2000b; *Trompert and Hansen*, 1998]).

(xi) The influence of an endothermic phase transition at 660 km depth in promoting episodic slab penetration or layering depending on the phase buoyancy parameter (e.g., [*Christensen and Yuen*, 1984; *Christensen and Yuen*, 1985; *Machetel and Weber*, 1991]), and possibly a secular switch from layered to whole mantle convection [*Steinbach et al.*, 1993].

(xii) The dynamics induced by continents, including episodic movements and the inherent instability of supercontinents to break up some characteristic time after forming, [*Gurnis*, 1988; *Lowman and Jarvis*, 1993; *Zhong* *and Gurnis*, 1993], and the different scaling of heat flux through continents and oceans [*Lenardic*, 1998].

(xiii) The ability of viscous dissipation to cause large heating locally [*Balachandar et al.*, 1993].

(xiv) Many results related to chemical mixing and thermochemical convection that are discussed later.

Additionally, a number of studies with time evolution have attempted to match specific observations, notable examples of which are the ability of convection constrained by plate motions over the last 120 Ma to match many but not all of the features observed in global tomographic models [*Bunge et al.*, 1998] and the ability of mantle flow history to match recent uplift rates in Africa[*Conrad and Gurnis*, 2003].

1.1. Problems and Limitations

Two major problems are faced by experimental studies, both of which cause uncertainty in how well the results apply to the real Earth. These are (i) uncertainty in the physical properties and parameters, and (ii) the effect of model simplifications, which are often made because it is not possible to treat, either numerically or in the laboratory, the full problem complexity.

1.1.1. Parameter Uncertainty

In many cases the important physical properties or parameters are uncertain enough that a range of behavior is possible. One notable example is the value of the Clapeyron slope of the spinel to perovskite+magnesiowüstite phase transition, estimates of which ranged from –2 to –6 MPa/K in the early 1990s [*Akaogi and Ito*, 1993; *Ito et al.*, 1990; *Ito and Takahashi*, 1989]- enough to cause a range in behavior from almost complete layering to basically whole mantle convection [*Machetel and Weber*, 1991; *Solheim and Peltier*, 1994; *Tackley et al.*, 1994]. The value is still uncertain with current estimates ranging from –0.4 to –2.0 MPa/K [*Fei et al.*, 2004; *Katsura et al.*, 2003]. Additionally, uncertainties remain in the depth of the majoritic-garnet to perovskite transition [*Ono et al.*, 2001], and in whether the ilmenite to perovskite transition [*Chudinovskikh and Boehler*, 2002] occurs in realistic mantle assemblages, both of which have significant effects on mass exchange between the upper and lower mantles.

Another notable uncertainty is the density contrast between subducted MORB, pyrolite, and depleted residue in the deep mantle, which is large enough that MORB could be either less dense or more dense than pyrolite in the deepest mantle [*Kesson et al.*, 1998; *Ono et al.*, 2001; *Ono et al.*, 2005]. This determines whether MORB settles into a layer above the CMB, which could have a large effect on geochemical observations [*Christensen and Hofmann*, 1994; *Xie and Tackley*, 2004a; *Xie and Tackley*, 2004b]. Another major example of uncertainty is the viscosity profile of the mantle, estimates of which are still changing (e.g., [*Forte and Mitrovica*, 1996; *Forte and Mitrovica*, 2001; *King*, 1995]). A final example of uncertainty is in how the thermal conductivity – particularly the radiative component – quantitatively varies with temperature and pressure [*Hofmeister*, 1999] which may have important effects on heat transport and thermal evolution [*van den Berg et al.*, 2001].

Some physical properties were not even known about until recently, particularly the post-perovskite phase transition [*Murakami et al.*, 2004; *Oganov and Ono*, 2004], which has important dynamical effects [*Nakagawa and Tackley*, 2004a; *Nakagawa and Tackley*, 2005b], and the spin transition in perovskite [*Badro et al.*, 2004], which has been argued to have a large effect on thermal conductivity, although the quantitative effect is extremely uncertain.

1.1.2. Model simplification

Models are necessarily simpler than Earth, both from a desire to study a well-constrained system where the effect of individual complexities can be clearly identified, but also because currently available numerical methods and computers are not capable of modeling the mantle/plate system with its full complexity. A major example of this is the difficulty in obtaining realistic plate tectonics in numerical models of mantle convection, which for many years necessitated inserting plates by hand and sometimes using rules for how they evolve. It is now established that simple pseudo-plastic yielding yields a crude approximation of plate tectonics in viscous flow models [*Moresi and Solomatov*, 1998; *Richards et al.*, 2001; *Tackley*, 2000b; *Trompert and Hansen*, 1998], yet these models have several shortcomings, such as double-sided subduction and no memory of previous weak plate boundaries, i.e., weak zones revert to the strength of pristine material once they become inactive. The latter may be important on the Earth as they can later be reactivated [*Gurnis et al.*, 2000]. Most likely a full visco-elasto-plastic treatment will be necessary to get realistic behavior, as hinted at by regional models (e.g., [*Regenauer-Lieb and Yuen*, 2003; *Regenauer-Lieb et al.*, 2001]).

Some other simplifications have come into focus recently, the first of which is the role of water, which has a strong effect on the viscosity [*Hirth and Kohlstedt*, 1996]. It has been argued, for example, that the deeper melting that would take place under mid-ocean ridges in a hotter mantle would generate a thicker rheological lithosphere, causing a negative exponent in the heat flux – Rayleigh number relationship [*Korenaga*, 2003]. A physical property that has so far been ignored in all global-scale convection models is grain size, which evolves with time and has a strong effect on the viscosity for diffusion creep. It has been argued that this might even cause a hotter mantle [*Solomatov*, 2001] or hot parts of the mantle [*Korenaga*, 2005] to be more viscous than average rather than less viscous as temperature-dependence would give.

Because of the uncertainties that ill-constrained parameters and model simplification introduce, it is important that modeling studies explore the full range of possibilities in order to establish which conclusions are robust and which depend on exact choice of parameter, and to also clearly identify the limitations and give appropriate caveats about applicability. Furthermore by determining which results match observations, parameters can be constrained (a type of 'inversion' by repeated forward modeling). Nevertheless, some proposed behaviors or mantle models can be ruled out even with our current knowledge, including some of the mantle models that have been proposed on the basis of geochemical observations [*Tackley*, 2000a].

Performing numerical experiments using a wide range of parameters carries an additional benefit that aids in our general understanding of Earth and its place in the pantheon of terrestrial planets. While only a particular parameter within the range studied may be relevant to Earth itself, other regions of parameter space allow us to examine how the variation of certain critical parameters gives rise to the great variety of behavior observed in the other terrestrial planets, both in our solar system and beyond, e.g. the control of lithospheric strength and convective vigor upon the occurrence of plate tectonics.

2. Thermo-chemical convection

2.1. Discussion and review

Reconciling geochemical and geophysical constraints on mantle structure and evolution remains one of the "grand challenges" in solid Earth science. There has been a recent resurgence of interest in this topic, and in thermochemical convection in general, due partly to seismological models that indicate the need for chemical variations in the deepest mantle [*Ishii and Tromp*, 1999; *Karato and Karki*, 2001; *Kennett et al.*, 1998; *Masters et al.*, 2000; *Trampert et al.*, 2004] and also partly to provocative proposals regarding mantle structure [*Becker et al.*, 1999; *Kellogg et al.*, 1999].

Several approaches are being taken to understanding the dynamics of thermochemical convection and how it is related to seismic, geochemical and other observations. One important topic is 'mixing', a term that is often used loosely to mean either the stirring and stretching of heterogeneities by convection (e.g., [*Christensen*, 1989a; *Ferrachat and Ricard*, 1998; *Gurnis*, 1986; *Kellogg and Turcotte*, 1990; *Metcalfe et al.*, 1995]), or the dispersion of initially nearby heterogeneities throughout the domain (e.g., [*Gurnis and Davies*, 1986; *Olson et al.*, 1984; *Schmalzl and Hansen*, 1994; *Schmalzl et al.*, 1995; *Schmalzl et al.*, 1996]).

The present discussion, however, focuses on studies where the chemical variations are active, i.e., affect the buoyancy, and often where tracking of specific trace elements is also performed. A typical investigative approach has been to insert a layer of dense material a priori and study the subsequent dynamics as it interacts with the convection (e.g., [*Christensen*, 1984a; *Davies and Gurnis*, 1986; *Hansen and Yuen*, 1988; *Hansen and Yuen*, 1989; *Olson and Kincaid*, 1991; *Schott et al.*, 2002; *Sidorin et al.*, 1998]), although [*Hansen and Yuen*, 2000] started with a linear chemical stratification. In the late 1990s, the field was envigorated by a number of developments, including a series of laboratory experiments that showed various hitherto unappreciated phenomena, particularly a 'doming' mode in which domes of material from a dense lower layer rise into the upper layer then fall, a process which can be repeated several times before large-scale overturn occurs [*Davaille*, 1999a; *Davaille*, 1999b; *Le Bars and Davaille*, 2002], by seismic inversions that found the bases of the large scale 'megaplumes' underneath the Pacific and Africa are dense [*Ishii and Tromp*, 1999], implying a chemical origin, and by a proposal that a dense, thick but strongly undulating layer exists in the bottom part of the mantle, helping to explain geochemical and seismological constraints [*Kellogg et al.*, 1999].

2.2. Three-Dimensional Experiments

Initial three-dimensional calculations of convection with an inserted dense layer comprising ~10% of mantle depth produced isolated 'ridges' or 'piles' separated by exposed CMB, with the 'piles' reminiscent of the seismically-imaged 'megaplumes', leading to the suggestion that these structures are thermo-chemical in origin [*Tackley*, 1998]. This is different from the globally-continuous layer comprising ~30% of mantle depth proposed by [*Kellogg et al.*, 1999] on the basis of geochemical mass-balance considerations. Numerical experiments with these different amounts of dense material were explored by [*Tackley*, 2002] and sample results are illustrated in Figure 1. When the dense material comprises 30% of mantle volume (Figure 1 left columns), a continuous undulating layer is formed, with hot upwellings rising from ridges of the dense layer. When the dense material comprises only 10% of mantle volume (Figure 1 right columns), it is swept into ridges separated by exposed patches of the CMB and again, hot upwellings rise from these ridges. The dense material becomes very hot because it is enriched in heat-producing elements (as either a primitive layer or a layer of segregated subducted oceanic crust would be) and heat must be transferred conductively across its interface (Figure 1(i)(k)(m)(o)). This causes very large lateral temperature variations in the deep mantle, probably causing very high amplitude seismic heterogeneity. It has been suggested that the thermal and chemical contributions to seismic velocity are of opposite sign and would approximately cancel out [*Kellogg et al.*, 1999]. The effect of this is explored in Figure 1(j)(l). Because the chemical boundary is sharp but the thermal boundary is diffuse, the boundary of the dense material will still cause high-amplitude heterogeneity, even at the nominal resolution of seismic tomography (Figure 1 (n)(p)). For intermittent ridges or piles this high-amplitude heterogeneity is at the base of the mantle, consistent with seismological models, whereas for a global layer it is in the mid-mantle, not consistent with tomographic models, as plotted using spectral heterogeneity maps in [*Tackley*, 1998]. Such matters are further explored in [*Deschamps et al.*, 2005].

This shows how numerical modeling can be used to compute the observational signatures of proposed mantle models for comparison with observations. Recently, such models have been extended to 3-D spherical geometry to determine the effect of viscosity contrast on the resulting thermochemical structures [*McNamara and Zhong*, 2004], and also to predict more specifically the form that chemical "piles" would take under Africa and the Pacific [*McNamara and Zhong*, 2005].

A limitation of all of these models is that a layer with a sharp interface is inserted a priori, which may or may not be reasonable as an initial condition for Earth [*Solomatov and Stevenson*, 1993]. Another method by which a layer might form is by segregation of subducted oceanic crust, if it is denser than regular mantle at deep mantle pressures.

2.3. Differentiation and Segregation

The feasibility of forming of a deep mantle layer by segregation of oceanic crust was shown by [*Christensen*, 1989b; *Christensen and Hofmann*, 1994]. In the latter work, the crust was generated by melting-induced differentiation of the mantle under mid-ocean ridges, something that has been seldom included in numerical studies, with some notable exceptions (e.g., [*Dupeyrat et al.*, 1995; *Ogawa*, 1997; *Ogawa*, 2000b; *Ogawa and Nakamura*, 1998; *van Thienen et al.*, 2004a; *van Thienen et al.*, 2004b; *van Thienen et al.*, 2005]). However, in the last several years our group has been experimenting with such models (first reported in [*Tackley and Xie*, 2002]), and these will be be discussed in the remainder of this paper.

When modeling thermo-chemical convection, care must be taken to include reasonable relative densities of the chemically-different components as a function of depth. In the models presented here, this is treated by having two reference states: one for the olivine system, and the other for the pyroxene-garnet system, the density profiles for which are illustrated in Figure 2 and discussed fully in [*Tackley and Xie*, 2003; *Xie and Tackley*, 2004a]. Of particular interest is the greater depth of the phase transition to perovskite in the pyroxene-garnet system, which causes subducted MORB to be buoyant in the range of approximately 660-720 km [*Ono et al.*, 2001], which has been proposed to have important dynamical effects [*Ringwood*, 1991]. In the experiments that follow, unmelted mantle ('pyrolite') is assumed to consist of 60% olivine and 40% pyroxene-garnet, while the extreme compositions are basaltic crust (C=1), which is pure pyroxene-garnet, and harzburgite (C=0), which is 6:1 olivine:px-gt. Melting occurs when the temperature exceeds a depth-dependent experimentally-based solidus, enough melt is generated to bring the temperature back to the solidus and the melt is immediately placed ('erupted') at the surface to form a crust. These calculations are intended to model the history of a terrestrial planet as it cools and radioactive elements decay, and thus have decaying radioactive heat sources and account for heat coming out of the core, either by assuming a simple heat capacity for the core (as in [*Steinbach et al.*, 1993]), or using a more sophisticated core heat balance (as in [*Buffett et al.*, 1996]). The models also include strongly temperature-dependent viscosity, with yielding in the lithosphere to prevent a rigid lid from forming.

2.4. Time Evolution and Post-Perovskite

Figure 3 shows a typical time-evolution for such a system with a deep mantle density contrast between harzburgite and MORB of about 2%, from [*Nakagawa and Tackley*, 2005b]. At early times, the upper mantle differentiates rapidly, but this is followed by whole mantle circulation. By the end of the experiment the mantle is extremely heterogeneous, containing 'blobs', stretched and folded strips of material, and a build-up of subducted crust above the CMB. This chemical structure is far more hetergeneous, and the interface of dense material at the base far less sharp, than in models in which a layer is inserted a priori. In some frames, subducted crust is trapped just below the transition zone, as also observed by [*Ogawa*, 2003], a topic that is returned to later.

These experiments also include the recently-discovered post-perovskite phase transition [*Murakami et al.*, 2004; *Oganov and Ono*, 2004], which has already been shown to have important dynamical effects- destabilizing the lower boundary layer hence resulting in more and smaller plumes and a higher mantle temperature [*Nakagawa and Tackley*, 2004a]. Regions of post-perovskite are shown in red, and many of the features predicted by [*Hernlund et al.*, 2005] can be seen. At early times when the core is hot, the CMB is still in the perovskite stability field, so a "double-crossing" of the phase boundary occurs, but once the core cools sufficiently it is blanketed by post-perovskite. In hot upwelling regions the post-perovskite layer is either non-existent (if the core is hot) or very thin. There is thus an anticorrelation between regions with a thick post-perovskite region and hot thermo-chemical "piles". Another effect is that due to the destablizing effect of the phase transition, a larger chemical density contrast is needed to stabilize a deep layer.

The post-perovskite phase transition provides an explanation for the seismic discontinuity at the top of D" [*Lay and Helmberger*, 1983] and the possible deeper discontinuity [*Thomas et al.*, 2004], and the presented models provide predictions about the relationship between these discontinuities and thermochemical "piles" that can be tested seismologically.

2.5. Stratification induced by phase transitions

The influence of the two-system phase transitions on isochemical or differentiating convection experiments is explored in Figure 4 (Tackley, P. J., EOS Trans. AGU, Fall Meeting Suppl. 2002). Almost all previously-published models of phase-transition modulated mantle convection (e.g., [*Christensen and Yuen*, 1985; *Machetel and Weber*, 1991; *Peltier and Solheim*, 1992; *Tackley et al.*, 1993;

Weinstein, 1993]) assumed a mantle made of 100% olivine, in which case (Figure 4 top left) the endothermic phase transition at 660 km depth causes a substantial inhibition of the radial flow, as indicated by the dip in the radial velocity profile. When, however, the composition is changed to pyrolite (Figure 4 top right), this inhibition becomes negligible, because the transition from garnet-majorite to perovskite is exothermic thus largely cancelling the effect of the endothermic spinel-to-perovskite transition. A possible intermediate transition to ilmenite [*Chudinovskikh and Boehler*, 2002] would reverse this picture and increase the layering [*van den Berg et al.*, 2002], but it is doubtful whether ilmenite occurs in a pyrolite composition (S. Ono, personal communication).

When chemical variations are added, the '660' regains its dynamical importance. It was previously found that the spinel-perovskite transition on its own might act as a chemical 'filter' [*Mambole and Fleitout*, 2002; *Weinstein*, 1992], but with both phase systems present the effect is magnified (Figure 4 second row). The vertical flow again exhibits a minimum at around 660 km, and there is also a local chemical stratification around 660 km, with enriched material trapped in the transition zone and depleted material trapped at the top of the lower mantle, as also observed by [*Fleitout et al.*, 2000; *Ogawa*, 2000a], but curiously, not by [*Christensen*, 1988]. This entrapment typically does not occur when a slab first encouters the region, but rather after the crust and residue components have separated in the deep mantle and are subsequently circulating as 'blobs'. Other features visible in the compositional field and its profile are a stable layer of segregated crust above the CMB, and a thin crust at the surface.

To demonstrate that this local chemical stratification around 660 km depth is due mainly to the different depths of the perovskite phase transition rather than deflection of transitions due to their Clapeyron slopes, a case in which all Clapeyron slopes are set to zero is presented (Figure 4 third row). In this case, the stratification is still strong, though somewhat diminished, showing that the depth separation on its own can cause significant chemical stratification, which phase boundary deflection adds to. Finally, when the perovskite phase transition is set to the same depth in both systems (Figure 4 bottom row), there is no flow restriction or chemical stratification around 660 km depth.

This local chemical stratification around 660-720 km is a prediction that could be tested seismically, which would help to determine whether the currently-estimated depths of these phase transitions are indeed correct.

2.6. Trace elements and geochemical modeling

A long-standing challenge has been to reconcile geochemical observations with a mantle flow model, and for this purpose it is important to track trace element evolution in mantle evolution experiments so that synthetic geochemiucal data can be generated and compared to observations, an approach that was pioneered by [*Christensen and Hofmann*, 1994], with other, more recent studies by [*Davies*, 2002; *Ferrachat and Ricard*, 2001; *Samuel and Farnetani*, 2003]. Experiments with passive tracers carrying trace elements have also been performed by [*van Keken and Ballentine*, 1998; *van Keken and Ballentine*, 1999].

Here, some recently published models by [*Xie and Tackley*, 2004a; *Xie and Tackley*, 2004b] are discussed. These models build on the earlier ones of [*Christensen and Hofmann*, 1994] by incorporating greater realism and by including the noble gases He and Ar in addition to U-Th-Pb and Sm-Nd systems. The most important ways in which realism is increased are a 4.5 Gyr run time instead of 3.6 Gyr, and a secular decrease in model activity due to the decay of radiogenic heat-producing elements and cooling of the mantle and core. Figure 5 illustrates how the chemical structure after 4.5 Gyr of evolution is dependent on the relative density of MORB in the deep mantle: when it is more dense (Figure 5(a)(d)(g)) a layer of segregated crust is formed, when it is of equal density a very thin transient layer of crust and residue is formed because the slab is cold (Figure 5(b)(e)(h)), and when it is buoyant a layer of residue is formed together with 'blobs' of crust in the mid mantle (Figure 5(c)(f)(i)).

The time evolution of heat flow and magmatism are plotted in Figure 6 (again from [*Xie and Tackley*, 2004b]). The total surface heat flow (thick solid line) decreases from about 100 TW to 20 TW over time, as expected, but conductive surface heat flow (thin solid line) is roughly constant. The discrepancy between these is made up by magmatic heat transport (dotted line), which is estimated to transport about 2 TW of heat in today's Earth, but if these models are reasonable, may have carried a lot more (up to 10s of TW) in the past. Indeed, it has even been proposed that magmatism transported most of the heat flux in a pre-plate-tectonic era [*Davies*, 1990; *Davies*, 1992; *van Thienen et al.*, 2004b], as is presently the case in Io [*Segatz et al.*, 1988]. The magmatic rate (Figure 6(b)) was substantially higher in the distant past, lying somewhere between the idealized models of constant at today's value (dotted line) and proportional to internal heating squared (dashed line).

The ratio $^3He/^4He$ plotted as a function of position (Figure 5(g)(h)(i)) shows the extremely heterogeneous nature of this model mantle. In these cases $^3He/^4He$ is low in former MORB because of the ingrowth of ^4He from U and Th (which are concentrated in MORB) and high in residue because it is assumed that He is more compatible (less incompatible) than U and Th [*Coltice and Ricard*, 1999]. However, the latter assumption is highly uncertain and its consequences are illustrated in the histograms of $^3He/^4He$ in Figure 7. When He is less compatible than U, both residue and crust develop a low $^3He/^4He$ signature, and high $^3He/^4He$ ratios (the peak at 35 Ra in Figure 7(a)) occur only in primitive, unmelted material. When, however, He is more compatible that U, the residue develops the highest $^3He/^4He$ ratios (Figure 7(b)), of up to 73 Ra. Figure 7(c) and (d) show the effect of calculating ratios over volumetric sampling cells, rather than considering each tracer as a sample (absolute abundance matters when summing over sampling cells). The difference is most dramatic for the 'less compatible' case, in which the peak is shifted to ~8 Ra, similar to that observed for MORB. Thus it is not surprising that material erupted in the last part of the experiment (Figure 7(e)) has a histogram that is similar to that observed for MORB, whereas for the 'more compatible' case the ratios are too high and too scattered (Figure 7(f)). [*Xie and Tackley*, 2004a] found that there is a trade-off with deep mantle crustal density, such that another MORB-like solution is obtained for buoyant crust and He equally compatible. These trade-offs need to be more thoroughly investigated.

The outgassing of radiogenic ^{40}Ar in these experiments is around 50%, similar to that observed in Earth, despite over 90% of 'primitive' nonradiogenic noble gases being lost [*Xie and Tackley*, 2004a]. This is possible because much of the outgassing occurs early on, when most of the final ^{40}Ar has not yet been produced.

Fractionation of U and Pb generates 'HIMU' in MORB, such that Pb-Pb diagrams develop a slope that for Earth corresponds to an isochron with an age of 1.5-2.0 Gyr [*Hofmann*, 1997]. In these numerical experiments, however, the slope is much larger (Figure 7(g)), corresponding to an isochron of 3.39 Gyr. This is because the signature is dominated by early-differentiating material, both because the melting rate was much higher early on and because this material has a more extreme signature in Pb-Pb space. [*Christensen and Hofmann*, 1994] obtained the correct slope because their model activity was constant with time and lasted for only 3.6 Gyr. [*Xie and Tackley*, 2004b] consider and test four hypotheses for the discrepancy between model and data: (i) HIMU was not produced early on, (ii) the melting rate is too low in these experiments, (iii) erasure of heterogeneities by stretching is not correctly treated, and (iv) the sampling lengthscale is inappropriate. It was found that sampling lengthscale affects only the scatter not the slope, the melting rate is reasonable (Figure 6(b)) although a higher rate would be acceptable, and a better treatment of stretching is helpful but probably cannot account for the whole discrepancy. The most effective way to resolve the discrepancy is for HIMU to not enter the mantle prior to about 2.5 Gyr before present (Figure 7(h)), which could be because trace elements were removed from the slab by melting prior to that time [*Martin*, 1986], or because of a change in atmosphere and ocean oxidation state [*Elliott et al.*, 1999].

2.7. Core and geodynamo evolution

Explaining how the heat flux out of the core can have stayed large enough over billions of years to maintain the geodynamo, without growing the inner core to a much larger size than observed, is a challenging problem. Parameterized models of core-mantle evolution in which no complexities are present predict a final inner core size that is much larger than that observed (e.g., [*Labrosse*, 2003; *Labrosse et al.*, 1997; *Nimmo et al.*, 2004]. As the heat conducted out of the core is determined by what is happening in the mantle, the time history of CMB heat flow is an important quantity to investigate using numerical models as it can provide an additional constraint on mantle models.

[*Nakagawa and Tackley*, 2004b] used a convection model similar to those already presented but with a parameterized core heat balance based on [*Buffett et al.*, 1992; *Buffett et al.*, 1996] to show that the presence of a layer of dense material above the CMB, either primordial or arising from segregated crust, substantially reduces the CMB heat flow hence inner core growth. The problem is, CMB heat flow can be reduced so much that it is insufficient to facilitate dynamo action, and can even become zero or negative. Because of this, a discontinuous layer, rather than a global layer, was found to be the most promising scenario. These tradeoffs are illustrated in Figure 8 (taken from [*Nakagawa and Tackley*, 2005a]), which shows the time evolution of CMB heat flow and inner core size from three calculations with different deep mantle density contrasts for subducted crust. When crust is neutrally buoyant (red curves), no dense layer builds up so CMB heat flow remains high and the inner core grows to over twice is observed radius. When crust is ~2% denser than pyrolite at the CMB (blue curves), a global layer builds up, eventually zeroing CMB heat flow and resulting in a slightly too small inner core. With an intermediate crustal density (~1% denser than pyrolite) the results are inbetween. [*Nakagawa and Tackley*, 2004b] found that it is difficult to match all constraints unless there is radioactive potassium in the core (e.g., [*Nimmo et al.*, 2004]), and mapped out the tradeoff between crustal density and core K content.

This is another example of the use of numerical experiments to constrain the values of uncertain physical parameters- in this case the potassium concentration in the core and the density contrast of MORB in the deep mantle.

3. Summary and Outlook

Mantle convection experiments play an essential role in understanding the dynamics, evolution and structure of Earth's mantle, and many fundamental findings have been established. A major problem is parameter uncertainty, which is sometimes large enough that seemingly opposite behaviors are possible, but many mantle models can be ruled out even with existing uncertainties. Most importantly, parameters can be constrained by comparing forward models to data, as has been demonstrated in this review using comparisons with seismic models, with geochemical data and with geodynamo history. The presented experiments also illustrate the fundamental importance of mineral physics data, particularly on phase transitions (including the recently-discovered post-perovskite transition) and the density as a function of composition and pressure.

This is an exciting time for mantle geochemistry, with new proposals being made and fundamental assumptions being questioned. For example, [*Ballentine et al.*, 2002] show that if current estimates for the helium flux out of the mantle are too high by a factor of three, then most of the paradoxes associated with He and Ar, including the 'need' for a layered mantle, would vanish. The idea that MORB and OIB could be derived from the same statistical distribution but with different sampling is explored by [*Ito and Mahoney*, 2005a; *Ito and Mahoney*, 2005b; *Meibom and Anderson*, 2004]. Water may cause the transition zone to act as a trace element filter [*Bercovici and Karato*, 2003]. A new way of modeling the sampling of a chemically-heterogeneous mantle with a heterogeneous size distribution has been developed [*Kellogg et al.*, 2002].

The coupled geodynamic-geochemical modeling approach reviewed here appears very promising, and there are some obvious improvements that could straightforwardly be made to the models, including three-dimensional spherical geometry, more realistic convective vigor, and higher resolution of the chemical heterogeneities (i.e., more tracers). 3-D geometry would, for example, allow a distinction to be made between OIB and MORB magmatism. Additionally, the sampling algorithm by which observed compositions are calculated from that carried on tracers, could be improved along the lines of [*Kellogg et al.*, 2002].

There are, however, several fundamental limitations that fall into the earlier-discussed category of 'model simplifications', even though the presented models may appear quite complex compared to previous models. Some examples are given: The slab processing (dehydration and migration of trace elements) that takes place in subduction zones may be very important for generating some geochemical signatures, but requires detailed, fine-resolution local models to treat properly (e.g., [*Ruepke et al.*, 2004; *van Keken et al.*, 2002]). The derivation of basalt composition from the source region may be more complicated than the simple partitioning assumed here [*Aharonov et al.*, 1997; *Donnelly et al.*, 2004; *Spiegelman et al.*, 2001]. Continents are geochemically important but are not included because the processes by which they form are too complicated and poorly understood to include in such global models, although some progress is being made on very early continent formation processes [*van Thienen et al.*, 2003; *van Thienen et al.*, 2004a]. Plate tectonics itself is only crudely represented, as a full treatment of rock rheology is beyond what is presently possible in global experiments. At this point, all of these complexities are essentially absorbed into the parameterization. The arguably important effects of water and grain size [*Bercovici and Karato*, 2003; *Korenaga*, 2003; *Solomatov*, 1996] are not treated. Accurate numerical treatment of entrainment is problematic [*Tackley and King*, 2003; *van Keken et al.*, 1997] so laboratory experiments are still useful (e.g., [*Gonnermann et al.*, 2002]).

Evaluating the effect of these and other complexities on the dynamics and observational signatures will keep geodynamic researchers and their coworkers in related fields busy for long into the future.

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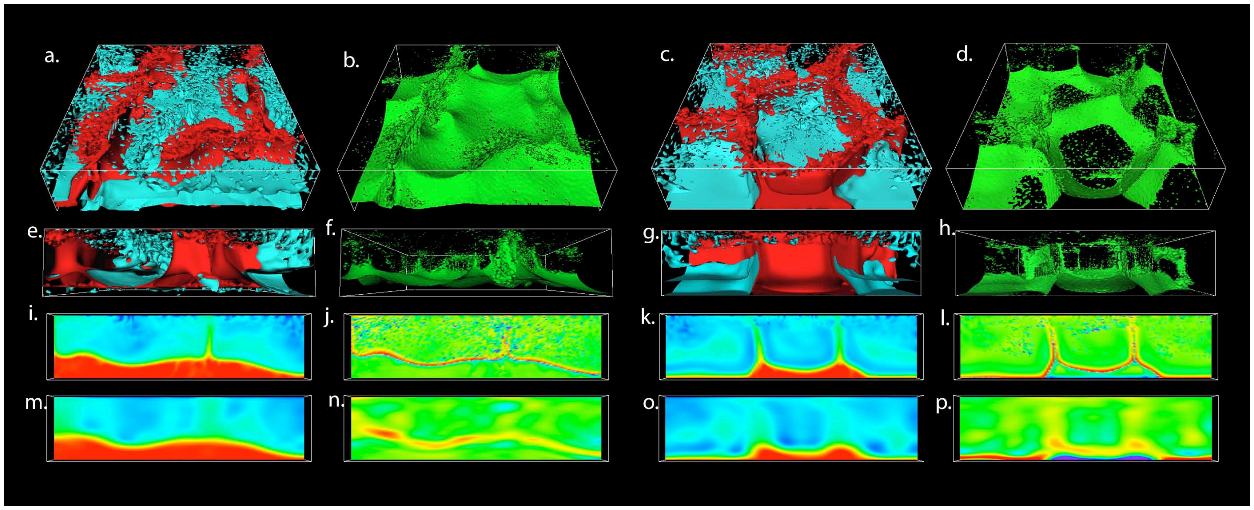

Figure 1. Three-dimensional thermo-chemical convection calculations from [*Tackley*, 2002]. The left two columns show a case with a dense layer initially occupying the lower 30% of the mantle volume, while the right two columns show a case with a dense layer initially taking up 10% of the mantle volume. (a)(e)(c)(g) Isocontours of residual temperature +-200 K, (b)(d)(f)(h) isocontours of composition=0.5, (i)(k) vertical cross-section of temperature field, which is filtered to the nominal resolution of seismic tomography in parts (m)(o) respectively, (j)(l) cross sections of T-0.75C, filtered in parts (n)(p) respectively.

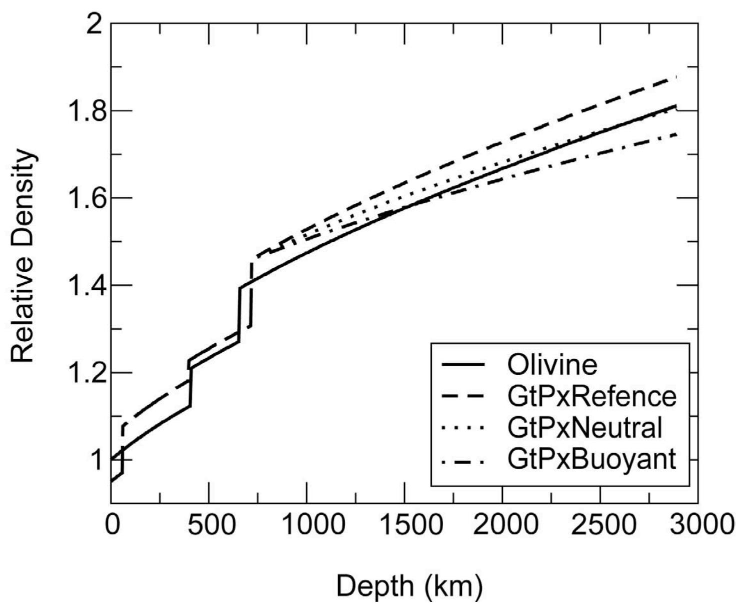

Figure 2. Reference state density profiles for the olivine and pyroxene-garnet components. For the latter, three different compressibilities are assumed in the lower mantle, leading to this component being either denser (GtPxReference), less dense (GtPxBuoyant) or the same density as the olivine component. As the slab contains a much higher fraction of the GtPx component then pyrolite, these relationships determine the relative density of MORB, residue, and primitive material.

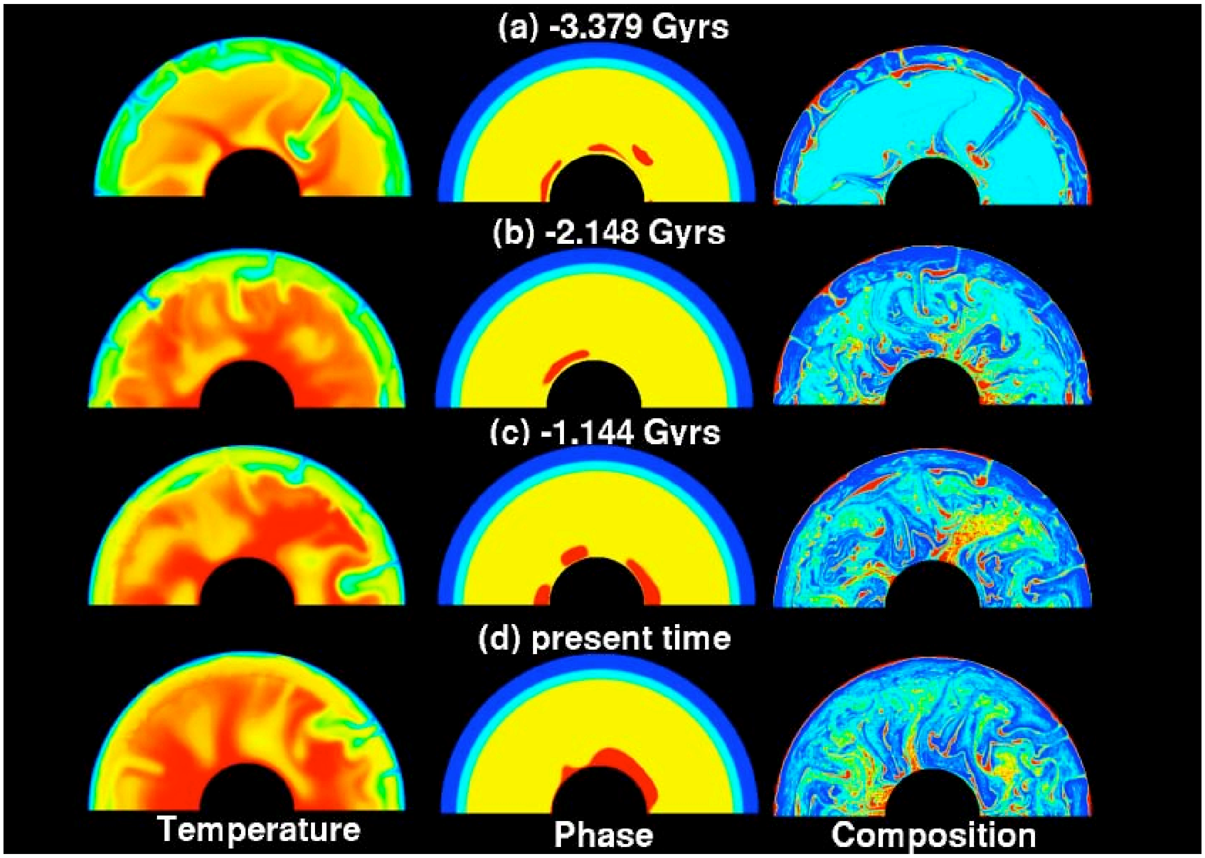

Figure 3. Time evolution of a model mantle with chemical differentiation and the post-perovskite phase transition, from [*Nakagawa and Tackley*, 2005b]. Left column: temperature. Center column: phase, where red=post-perovskite and the other colors are the usual mantle phases. Right column: composition, from red=crust to dark blue=harzburgite. Times are as indicated.

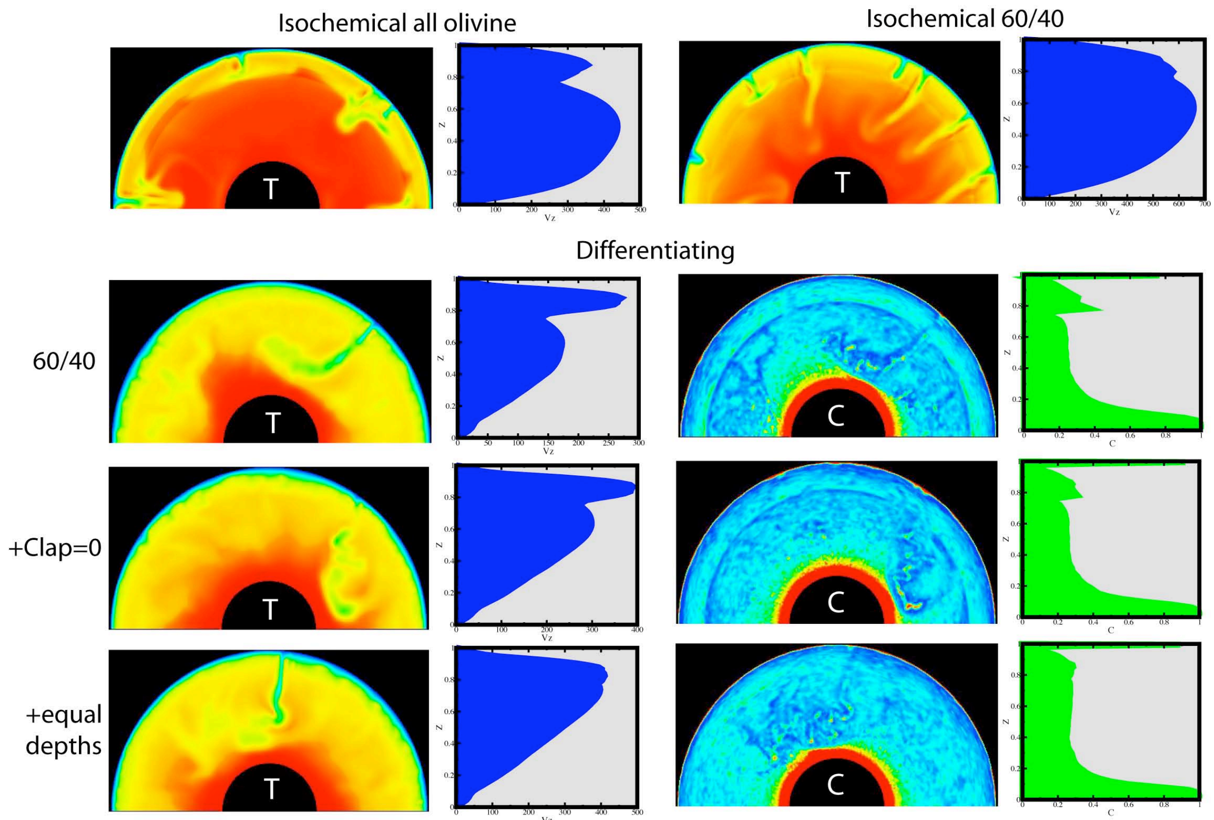

Figure 4. Effect of phase transitions on layering of flow and average composition, from two-dimensional calculations in a half cylinder. Plots show 2-D distributions of superadiabatic temperature (labeled 'T'), composition (labeled 'C') varying from red=crust to dark blue=residue, the time-averaged mean of the modulus of radial velocity (blue graphs) or the horizontal average composition (green graphs). Top row: isochemical cases with either (left) 100% olivine or (right) 60% olivine and 40% pyroxene-garnet; the remaining cases include chemical differentiation. Second row: 100% olivine. Third row: 60% olivine, 40% pyroxene-garnet. Fourth row: 60/40 with zero Clapeyron slopes. Bottom row: 60/40 with zero Clapeyron slopes and the transition to perovskite set to an equal depth for both systems.

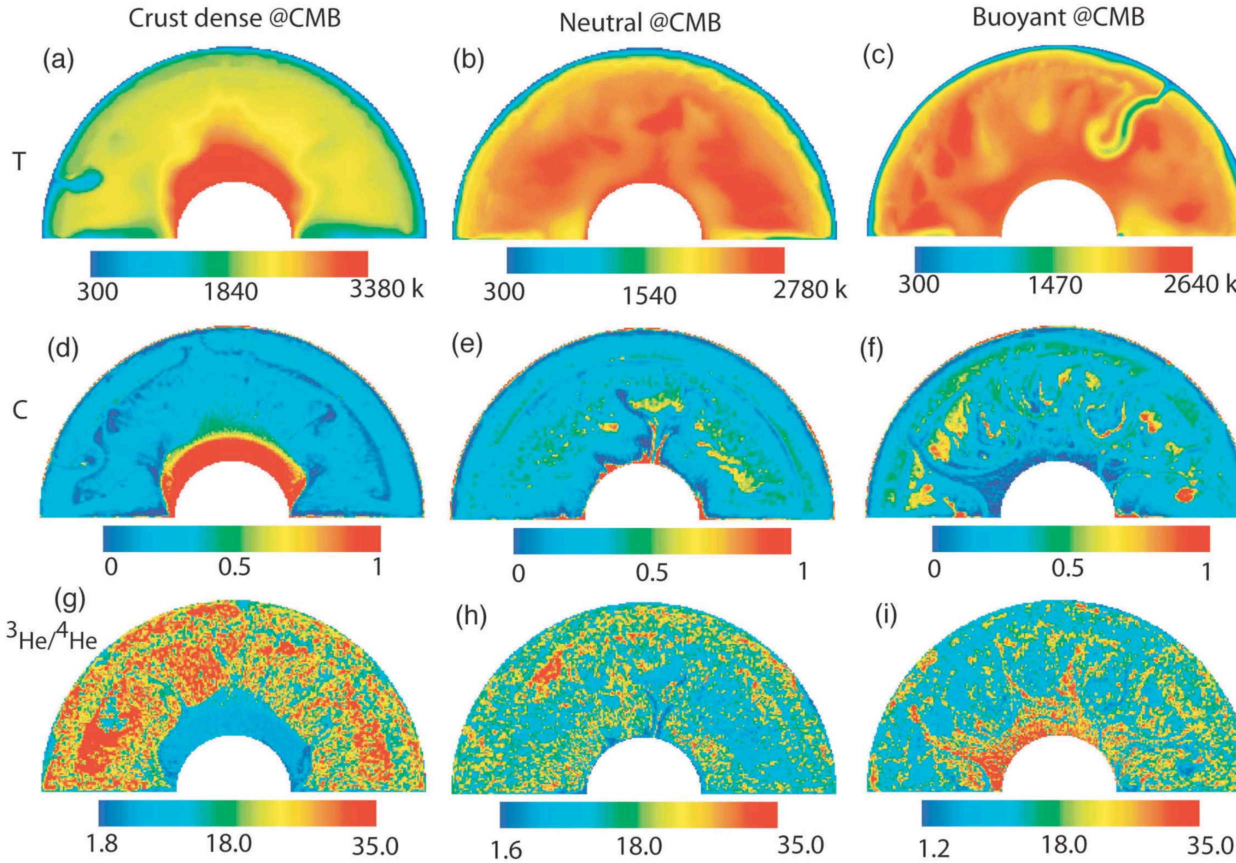

Figure 5. The effect of deep-mantle MORB density of mantle thermo-chemical structure including helium ratios, from [*Xie and Tackley*, 2004a]. (a)(b)(c) temperature, (d)(e)(f) composition, and (g)(h)(i) 3He/4He. (a)(d)(g) PxGt system (hence MORB) dense at the CMB, (b)(e)(h) PxGt system neutrally dense at the CMB, (c)(f)(i) PxGt system less dense at the CMB.

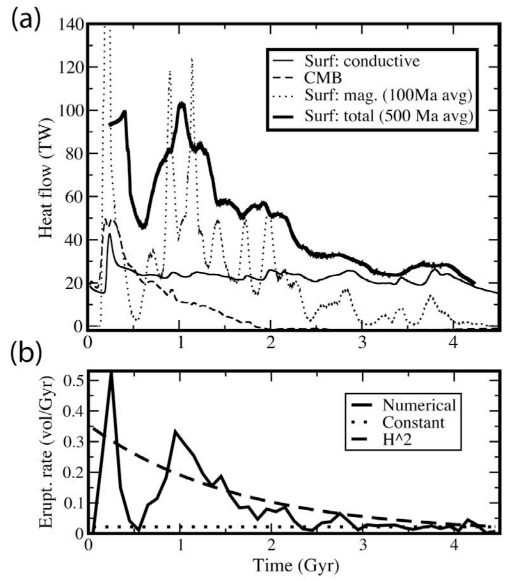

Figure 6. Time evolution of various diagnostics from a typical case in [*Xie and Tackley*, 2004b]. (a) Surface and CMB heat flow scaled to a spherical planet, showing CMB (dashed), surface conductive (solid), surface magmatic (dotted), and surface total (bold indicates averaging over a 500 Myr sliding window). (b) Crustal production (eruption) rate in mantle volumes per Gyr, averaged over three representative cases in 100 Myr bins, and compared to theoretical models (dotted and dashed lines).

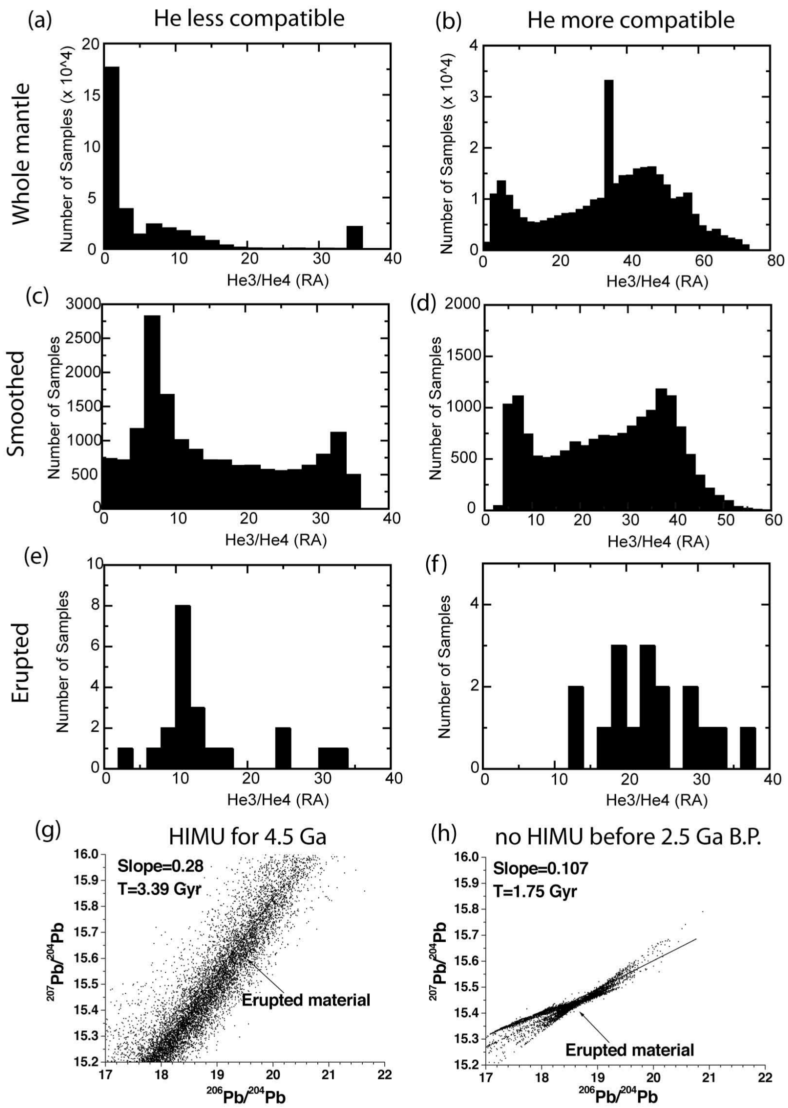

Figure 7. Isotope diagrams for various cases with chemical differentiation and tracking of trace elements. (a)-(f) Histograms of $^{3}He/^{4}He$ from [*Xie and Tackley*, 2004a]. A case in which He is less compatible (more incompatible) than U is plotted in (a)(c)(e) while a case in which He is more compatible than U is plotted in (b)(d)(f). Histograms are counting either individual tracers (top row (a)(b)), sampling cells (second row (c)(d)) or material erupted over the last 200 Ma (third row (e)(f)). (g)(h) $^{207}Pb/^{204Pb}$-$^{206}Pb/^{204}Pb$ diagrams from [*Xie and Tackley*, 2004b]. (g) is for a case in which high U/Pb (MU) material is subducted throughout the modeled history, whereas (h) is for a case in which HIMU material is subducted only for the last 2.5 Gyr of the model time.

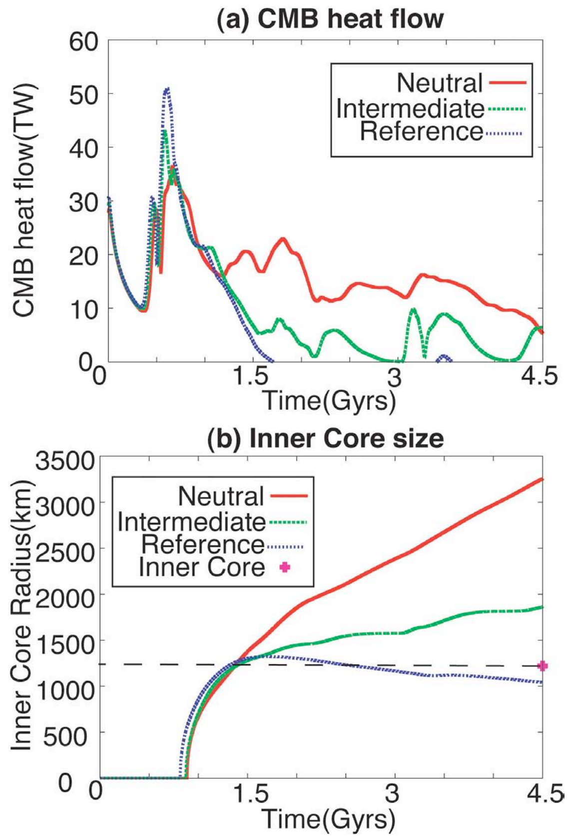

Figure 8. Time evolution of CMB heat flow and inner core size from the numerical convection calculations of [*Nakagawa and Tackley*, 2005a] with chemical differentiation and three different density contrasts for MORB in the deep mantle.