



2048-8

From Core to Crust: Towards an Integrated Vision of Earth's Interior

20 - 24 July 2009

Simulating the thermal and chemical evolution and structure of Earth's mantle and core

P. Tackley Inst. of Geophysics, ETH Honggerberg Switzerland

Simulating the thermal and chemical evolution and structure of Earth's mantle and core

Paul J. Tackley

Takashi Nakagawa ETH Zürich





Interdisciplinary approach to Earth/planetary dynamics



Escapes











Figure 16 Three-dimensional projection of $^{87}\mathrm{Sr}/^{86}\mathrm{Sr},$ $^{143}\mathrm{Nd}/^{144}\mathrm{Nd},~^{206}\mathrm{Pb}/^{204}\mathrm{Pb}$ isotope arrays of a large



Geochemical cartoon models: which ones "work" both geophysically and geochemically?



example (end results of 4.5 Gyr evolution)



0.0%

1.8%

3.6%

Approach: Numerical modelling of coupled systems

- Mantle+Plates: Visco-plastic fluid dynamical model
- Geochemistry: Particles track composition. Melting causes crustal formation & trace element fractionation.
- Core: Parameterized heat balance/evolution
- Mineral physics: Solid-solid phase transitions coupled to composition, depth-dependent material properties, ...

Ingredients: Physics

- Compressible anelastic (physical properties depend on depth)
- Viscosity dependent on:
 - Temperature
 - Depth (typically factor 10 with depth + jump @660)
 - Stress (yielding gives plate-like behaviour)
- Multiple phase transitions (including post-perovskite)
- Internal heating + cooling core
 - Parameterized core energy balance similar to Buffett's (Nimmo's gives similar results)
- Cylindrical geometry (2-D) or 3-D spherical.

Ingredients: Chemistry

- Major elements:
 - 2-components: 'crust' (basalt/eclogite)<-> 'residue' (harzburgite).
 - Solidus (<u>Herzberg et al 2000; Zerr et al 1998</u>); melt instantly removed to form surface crust.
 - Chemical density variation depends on depth (2-component system)
- (in some studies: Trace elements:
 - ²⁰⁷Pb, ²⁰⁶Pb, ²⁰⁴Pb, ¹⁴³Nd, ¹⁴⁴Nd, ¹⁴⁷Sm, ²³⁵U, ²³⁸U, ³He, ⁴He ³⁶Ar, ⁴⁰Ar, ⁴⁰K, ²³²Th
 - Initial concentrations represent mantle after extraction of CC.
 - Unmelted material would have ³He/⁴He=35 today.
 - Radioactive decay
 - Partitioning between crust + residue on melting. Coefficients from (Hofmann 88) and variations on (Hiyagon+Ozima 86)
 - Noble gases outgas on eruption (outgassing fraction 90% in presented models))
- Homogeneous start

Numerically modeling mantle thermochemical evolution: like baking a cake

o Ingredients

- o Physical & chemical properties & behaviors (mineral physics, rheology, partition coefficients, melting, etc.)
- o Initial condition (homogeneous? layered?)

o Baking method (computer 'oven')

- o Convection calculations with geochemical tracers
- o Need to run for billions of years for geochemistry

o Outputs: what type of cake?

- o Geophysical: compare structure to seismology, heat flow & T vs. time, core evolution...
- Geochemical: Layering, isotope ratios (³He/⁴He distributions etc.), outgassing, heterogeneity lengthscales, etc.
- o **Hypothesis testing**: which mantle models are consistent with both geochemical and geophysical constraints?

Numerically-intensive calculations







Volume 361 No. 6414 25 February 1993 \$7.75



15 years of progress



Avalanches in the mantle

1993: supercomputer, spectral code

2008: laptop, multigrid code

to technology

Geochemical cartoon models: which ones "work" both geophysically and geochemically?







Trace element ratios are heterogeneous!



General structure and evolution

- Highly heterogeneous in major- and traceelements
- Build-up of "messy" basal layer
- >95% has differentiated- very little primitive 'pyrolite' - rather mixture of MORB and depleted compositions



Outline

- Introduction. General evolution
- Transition zone and below
 - Dynamically-induced chemical stratification around 660 km
- Deep mantle
 - Does subducted MORB settle @ CMB?
 - Chemical stratification of the lower mantle
 - How does this affect the evolution of the core/dynamo?
 - Relationship between seismic tomography & CMB heat flow variations
 - Dynamical implications of post-perovskite transition
- Future prospects and Summary

Different depths of perovskite transition in olivine and pyroxene systems



From Ita and Stixrude

Transition zone

- 'old' numerical models assume mantle is 100% olivine and get significant effect of 660 km phase transition, but actually
 - it's only ~60% olivine
 - Current estimates predict fairly weak Clapeyron slope for 660 km phase change
- Composition-dependence of phase change to perovskite around 660-750 km depth can have a large effect!

Phase change "filter effect" on chemical heterogeneity

MORB density inversion below 660 km

• from Ringwood

Ono et al 2001



Phase change "filter effect" a. Endothermic transition



b. Deeper MORB transition



Comparison of Ol-only and combined phase systems



T. Nakagawa, B.A. Buffett / Earth and Planetary Science Letters 230 (2005) 11-27

Analysis of this

Tackley et al. 2005



TZ Conclusions

- Purely thermal convection: ~minimal layering with both phase systems included
- +chemical variations: Different depths of perovskite transition in olivine and pyroxene systems leads to partial layering of flow and composition
- Recent mineralogical-seismological study of Cobden, Goes, Cammarano, Connoly (GJI 2008) finds MORB enrichment in TZ and depletion below 660



How dense is MORB near the CMB?

- Ringwood 1990: 2-4% denser throughout lower mantle (110-220 kg/m³ @ cmb)
- Kesson 1998: 30 kg/m³ less dense than pyrolite, 11 kg/m³ denser than depleted residue
- Ono et al 2001: less dense than pyrolite in deep mantle
- Guignot & Andraut 2004: 25-95 kg/m³ denser
- Hirose et al 2005: 200-300 kg/m³ denser throughout lower mantle (3.5-5.3% @CMB)

Assumed density profiles: composition-dependent mineralogy





Average chemical stratification in the lower mantle

Why does chemical stratification develop?

- 1. Gravitational settling
 - a. MORB segregation at the CMB [Christensen and Hoffmann, 1994]. Uncertain density contrast of MORB in deep mantle.
 - b. Depletion of uppermost mantle [Ogawa, Davies]
- 2. Phase transitions "filter effect"
 - a. Endothermic: partially traps denser material (MORB) in lower mantle [Weinstein 1992; Mambole+Fleitout 2002]
 - b. Multi-component: MORB transforms deeper: partially traps MORB in the transition zone, depleted material @ top of lower mantle [Ogawa, Xie/Nakagawa+me, Mambole+Fleitout unpublished]

Analyze radial T and density profiles



Nakagawa & Tackley 2005 gcubed

INSERT GRAPHS



Superadiabatic T profile is preferred from recent inversions



Jan Matas (talk @ Munich 2006)

Saskia Goes (talk @ Munich 2006)

2000

temperature (°C)

3000

Tmelt

outer core

4000

Tpot mantle

T phase

constraints adiabat

1000

seismic

transition
Summary: gravitational settling

- Density contrast of MORB seems large enough to get substantial settling
- Can lead to superadiabatic T and density profiles

What effect does this have on core evolution?

Mantle convection determines the heat flux out of the core

Core/geodynamo evolution

•Heat flux out of the core must be

- •Large enough for geodynamo to exist for billions of years
- •Small enough that inner core doesn't grow to larger than observed

A layer of dense material above the CMB has a strong effect on core thermal evolution

Simulated mantle + parameterised core

- Core param. is similar to Buffett's. Nimmo's gives similar results
 - Nakagawa, T. and P.J. Tackley, Effects of thermochemical mantle convection on the thermal evolution of the Earth's core, Earth Planet. Sci. Lett., 220, 107-119, 2004
 - Nakagawa, T., and P. J. Tackley, Deep mantle heat flow and thermal evolution of the Earth's core based on thermo-chemical multiphase mantle convection, Geophys. Geochem. Geosys, 6, Q08003, doi: 10.1029/2005JB003751, 2005.

T. Nakagawa, P.J. Tackley / Earth and Planetary Science Letters 220 (2004) 107–119



Fig. 2. Time evolution for passive-composition (B=0) cases (isochemical and differentiating). (a) Temperature at CMB. (b) Radius of the inner core. (c) Heat flux through the CMB. (d) Heat flux through the surface. The dotted line in (c) shows the heat flux required to maintain the magnetic field by geodynamo action. The large asterisk symbol in (b) and (d) shows the presentday inner core radius and heat flux obtained from observational data, respectively.

112

b. primordial layering



Fig. 4. Structural evolution for layered start cases. (a) B = 0.12. (b) B = 0.24. The top row in both (a) and (b) shows the temperature field and the bottom row shows the compositional field. Red: high temperature and composition. Blue: low temperature and composition.





Fig. 3. Time evolution for the layered start cases. (a) Temperature at CMB. (b) Radius of the inner core. (c) Heat flux through the CMB. (d) Heat flux through the surface.

c. layer builds up through melt-induced differentiation



Fig. 6. Structural evolution for differentiating, homogeneous start cases. (a) B=0.12. (b) B=0.24. The top row in both (a) and (b) shows the temperature field and the bottom row shows the compositional field. Red: high temperature and composition. Blue: low temperature and composition.



Fig. 5. Time evolution for differentiating, homogeneous start cases. (a) Temperature at CMB. (b) Radius of the inner core. (c) Heat flux through the CMB. (d) Heat flux through the surface.

Summary

- No layer: too large CMB flux & inner core
- Primordial layer: good!
- Layer that grows with time: more difficult to satisfy constraints
- How about adding K in core? NEXT



CMB heat flow either drops to zero (global layer) or inner core grows too big!

Nakagawa & Tackley, Gcubed 2005



Radioactive K in core seems necessary



Outline

- Introduction. General evolution
- Transition zone and below
 - Dynamically-induced chemical stratification around 660 km
- Deep mantle
 - Does subducted MORB settle @ CMB?
 - Chemical stratification of the lower mantle
 - How does this affect the evolution of the core/dynamo?
 - Relationship between seismic tomography & CMB heat flow variations
 - Dynamical implications of post-perovskite transition
- Future prospects and Summary

Large LATERAL VARIATIONS in CMB flux – influence dynamo



Histograms



Nakagawa & Tackley, 2008

Outline

- Introduction. General evolution
- Transition zone and below
 - Dynamically-induced chemical stratification around 660 km
- Deep mantle
 - Does subducted MORB settle @ CMB?
 - Chemical stratification of the lower mantle
 - How does this affect the evolution of the core/dynamo?
 - Relationship between seismic tomography & CMB heat flow variations
 - Dynamical implications of post-perovskite transition
- Future prospects and Summary

Dynamical Implications of the Post-Perovskite phase transition

New (2004) phase change discovered near the coremantle boundary



Fig. 3. High P-T phase diagram of MgSiO, predicted by first principles calculation based on the local density approximation (LDA) and generalized gradient approximation (GGA) [Tsuchiya et al., 2004b]. The lower and upper bounds were determined from LDA and GGA calculations, respectively. The calculated Clapeyron slope is about 7.5 MPa/K. The dashed line is the phase boundary proposed by combining data of the experimental transition condition (red star) [Murakami et al., 2004] and the Clapeyron slope assumed to explain the D* topography by solid-solid phase change [Sidovin et al., 1999]. The vertical shaded bound is the pressure range across the D* topography. The schematic Earth cross section demonstrates the correspondence of the Earth's structure and the post-perovskite phase transition.

Lay et al.[2005 in EOS]

Perovskite to post-perovskite

Pressure: approximately 120 GPa (2700km) Clapeyron slopes: +3 to +13 MPa/K

Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004.

Transition from double to single phase boundary



- Cold CMB => Single crossing
- Hot CMB => Double-crossing or no crossing (No PPV in hot plumes)

PPV transition promotes: Smaller-scale plumes, hotter mantle Nakagawa and Tackley[2004, GRL]



3D Spherical: Plumes also affected but more difficult to characterize

no PPV

h0=75 km

h0=300 km



Tackley, Nakagawa, Hernlund, 2007

Spherical cases





(Nakagawa & Tackley, 2005)



Spherical: also similar (end results of 4.5 Gyr evolution)



0.0%

1.8%

3.6%

PPV has strong influence on deep mantle seismic heterogeneity

- Large: "Lay discontinuity" Vs~2%
- Sharp-sided structures
- Lateral variations in PPV depth => largeamplitude lateral seismic heterogeneity



(Nakagawa & Tackley, 2005)

Lateral spectrum of Vs @ 2700km, 3-D cases



PPV effect can be larger than T & C! Composition has a flatter spectral slope

PPV: summary

- Slight destabilization of hot lower thermal boundary layer; destabilizes chemical layering
- Slight mantle T rise, depending on (T,p) location of PPV transition
- Anticorrelation between regions of thick PPV and hot, chemically-dense "piles" assuming C-independent PPV parameters
- Large effect of deep mantle seismic anomalies

Possible structures above CMB



Cartoon by John Hernlund

Current direction: Self-consistent mineralogy

Complicated phase relationships of mantle materials Hirose [2002]

MgSiO₃



Figure 1. Majorite-perovskite transitions in different bulk compositions; majorite-perovskite transition in MgSiO₃ [*Hirose* et al., 2001b], Mg-perovskite-in and majorite-out curves in pyrolite (this study) and mid-ocean ridge basalt (MORB) [*Hirose* et al., 1999], and gamet-perovskite plus corundum transition in Mg₃Al₂Si₃O₁₂ [*Hirose et al.*, 2001a]. The dashed lines indicate the postspinel phase boundary in pyrolite. Note that majoriteperovskite transition pressures are strongly dependent on the chemical composition, contrary to the postspinel phase boundary.

Mg₂SiO₄



Figure 3. Phase boundaries in Mg₂SiO₄ determined in this study. The solid and shaded symbols are based on the *Jamleson et al.*'s [1982] and *Anderson et al.*'s [1989] gold pressure scales, respectively. The postspinel phase transition pressure based on the Jamieson et al.'s scale matches with the depth of the 670-km seismic discontinuity. The dashed lines indicate the postspinel phase boundary in pyrolite from Figure 4.

Mantle material: Complicated phase relationship under various P and T conditions

Parameterised approach



Input: Density jump and CS due to phase transitions into depthdependence along with adiabat

Simplifying other complicated phase (e.g. Wadsleyite-Ringwoodite, Two phases of Garnet (Majorite and Akimotite)

Effects of more complicated phase relationship for mantle minerals in numerical mantle convection model ???

Generating realistic phase assemblages computationally

Determined by Free Energy Minimization technique: PERPLEX [Connolly, 20051 Harzburgite

$$G(T,P) = \sum_{i} n_i(T,P) \mu_i(T,P)$$

Data for components for two materials from [Stixrude and Lithgow-Bertelloni, 2005]



kam^-3 5500

5000

4500

4000

3500

4500

Component	Harzburgite	MORB	MORB	MORB	
	(mol%)	(mol%)	2500		
${ m SiO}_2$	36.04	41.75	 tig 2000		
MgO	57.14	22.42	[●] 1000 500 [●]		
FeO	5.41	6.00	0 1500 3000	3000	
CaO	0.44	13.59	Temperature(K)		
Al_2O_3	0.96	16.24	Solid line: Solidu	JS	

Reference density along with adiabat



Pyrolite: Combined two component via amount of MORB composition

Density difference @ CMB
2.7% between Harzburgite and MORB (PERPLEX)
3.6% (Linearized)
2.16% between MORB and Pyrolite (PERPLEX)
=2.32% (Linearized)

Olivine-WadsleyiteRingwoodite-Perovskite-pPv
Px-gt(il or ak)-pv: gradual
-pPv: close to CMB (2800km
depth ?)
Linear

PERPLEX



Time for the CONCLUSIONS

Numerical mantle convection calculations are a good way of integrating observations & measurements from various fields

- Mineral physics
- Seismology
- Geochemistry
- Paleomagnetism, core dynamics
- (geology, tectonics, etc.)

Important points

- Mantle is heterogeneous at all lengthscales.
 - chemical effects important
 - PPV has strong effect in deepest mantle
- Expect average chemical stratification of the mantle, due to combination of phase transitions and gravitational settling
- Effects on the geodynamo/core:
 - Settling of basalt at the CMB influences heat flux
 - Preferred solution: Intermittent piles and some K in core
 - Strong lateral variations in cmb heat flux
 - Vs-flux relationship is nonlinear and influenced by PPV and chemical variations
- PPV has small dynamical influence, slightly destabilises lower boundary layer
- Many of these depend strongly on uncertain mineral physics parameters!

Uncertain mineral physics parameters strongly affect results

- Density of MORB at CMB pressures

 Structure & core evolution
- Post-perovskite phase change parameters
 - Clapeyron slope (-7? -13?), compositiondependence, width
- Composition-dependent phase changes around 660 km depth.

Summary diagram





For more information

 http://www.gfd.geophys.ethz.ch/%7Epjt/ bibliography.html