Convective vigour and heat flow in chemically differentiated systems

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SUMMARY

Parametric models of planets used to study their thermal evolution are generally based on scaling laws for purely thermal convection. However, planetary mantles may be chemically highly differentiated due to partial melting, which may form thick layers of depleted and dehydrated melting residue (e.g. continental roots). This results in inhomogeneity of density, which affects the driving force of convection, and viscosity (through the water content), which directly influences the dynamics of the system.

This work investigates the applicability of scaling laws developed for purely thermally convecting systems to chemically differentiated systems representative of planetary mantles. The effects of depletion related buoyancy and melting related dehydration, and particularly the stratified convection patterns which may result from these, are considered. Two different strategies are applied to this end. First, a large number of numerical thermochemical convection experiments are performed, of which the dynamics and heat flow characteristics are studied. Secondly, theoretical approximations are developed from existing scaling laws to describe the heat flow of chemically stratified systems with separately convecting layers. These are tested using numerical simulations.

The results show that the presence of a chemical stratification in the mantle may significantly alter heat flow patterns relative to a purely thermally convecting system by either influencing the thickness of the thermal boundary layer or dividing the convecting part of the system in vertically separate cells. This is consistent with recent petrological findings. Although the chemical stratification may be inherently instable against remixing, the present results suggest that the timescales of remixing may be much larger than those of thermal equilibration. Therefore, it is important to consider chemical stratification in thermal evolution models.

For present-day Earth conditions and realistic rheological parameters, the results predict that the lower parts of continental roots may be convecting separately from the underlying mantle. The thick depleted layer which has been speculated to underly the martian crust may also have exhibited convection in the lower parts. When convection takes place in the depleted zone, mantle heat flow values are predicted to increase by a factor of 2–5 relative to non-convecting depleted zones. If this process acts for significant periods of time during planetary evolution, it will strongly influence the planet's thermal evolution.

Key words: heat flow, mantle convection, mantle rheology.

1 INTRODUCTION

Scaling laws for Earth's surface heat flow as a function of mantle temperature have been around for nearly 40 years now (Turcotte & Oxburgh 1967), and have helped us understand the thermal evolution of the terrestrial planets (e.g. Schubert *et al.* 1980; Christensen

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1985). In more recent years, the original versions which were devised for isoviscous systems have been replaced by more complex scaling laws which are applicable to systems with temperature dependent and non-linear rheologies (e.g. Solomatov 1995; Reese *et al.* 1998, 1999). However, the purely thermal nature of the buoyancy consideration in these scaling laws requires some caution in their application to the thermochemical convection systems of the planetary mantles.

It has become more and more clear that chemical differentiation of a planetary mantle resulting from partial melting may result in a density stratification which may profoundly influence the dynamic evolution of the mantle (Oxburgh & Parmentier 1977; Sleep & Windley 1982; Vlaar & Van den Berg 1991; Parmentier & Hess 1992; Van Thienen *et al.* 2004; Zaranek & Parmentier 2004). In addition to this, it is predicted that the effect of water and dehydration during partial melting (e.g. Hirth & Kohlstedt 1996) can have a significant influence on mantle dynamics and, therefore, mantle cooling as well (Korenaga 2003; Lee *et al.* 2005).

Important examples of chemically distinct regions in Earth's upper mantle are continental roots. These are seismically imaged to depths of several hundred kilometres (Grand 1994; Trampert & Woodhouse 1996; Fischer & Van der Hilst 1999), and generally a chemical density reduction due to depletion is invoked to (partially) explain their stability (see King 2005). Numerical models of the martian mantle also predict a depleted layer of several hundred km thickness underneath its thick crust (Schott *et al.* 2001). Parametric models for the thermal evolution of Venus including chemical differentiation by Parmentier & Hess (1992) show the formation of a 100–200 km thick depleted layer in the uppermost mantle as well.

The purpose of this work is to investigate the effect of chemically induced density (depletion) and viscosity (dehydration) anomalies on the convective vigour and heat flow of bottom heated convective systems in order to study the applicability of classic scaling laws and find modifications of these which will increase their applicability to the chemically heterogeneous mantles of the terrestrial planets. The chemically induced changes in density are expected to be generally no more than a few percent and, therefore, probably not directly important for the convective vigour, as the Rayleigh number scales linearly with density. However, chemical inhomogeneities may cause a stratification in the mantle of material. Under certain conditions, this may result in separate convection cells in the different layers. For example, the numerical models of De Smet et al. (1998) dealing with the formation and evolution of continental roots show long-term stability of the chemical stratification (depleted root and undepleted mantle) as well as separate convection in the root and the underlying mantle. Recently, results from petrological studies consistent with convective patterns in continental roots have been published as well (Drury et al. 2001; Spengler et al. 2006).

Earlier work by McNamara & van Keken (2000) has shown that layered convection significantly reduces the heat flow relative to single layer convection. Though their subject of interest was Earth's entire mantle, the results apply equally to other convecting systems within Earth's upper mantle. Lenardic & Moresi (2003) studied the thermal characteristics of convection underneath a conducting lid that was partially or completely covering the convecting fluid.

In this paper, two different approaches are applied to investigate the importance of dehydration related viscosity stratification and chemical buoyancy related flow stratification. First, I have run a large number of numerical thermochemical convection experiments with an initial phase of differentiation by partial melting, followed by a long period (0.5–1.5 thermal diffusion times h^2/κ) during which the distribution of the chemical heterogeneities as well as the convective vigour and surface heat flow were monitored. The model space is mapped for a range of values of the Rayleigh number, dependence of viscosity on temperature and water content, and implicitly on the degree of differentiation. Secondly, the subject is approached starting from existing scaling laws for convection in isoviscous and temperature and strain-rate dependent rheology systems by applying these to stratified systems. In order to better understand the results of this scaling law approach, a number of numerical stratified thermal convection experiments are performed which closely match the settings represented by the scaling law models. Finally, a synthesis is made of the strategies, and the implications of the results to the terrestrial planets are discussed.

2 NUMERICAL THERMOCHEMICAL CONVECTION EXPERIMENTS

A finite element code based on the commercial package SEPRAN (Segal & Praagman 2002) including partial melting (Van den Berg *et al.* 1993; Van Thienen *et al.* 2003) is used to numerically investigate the evolution of chemically differentiated systems over timescales of 0.5–1.5 thermal evolution times (h^2/κ) . Specifically of interest are one or more periods of (near) statistical steady state in terms of mantle temperature, convective vigour, and distribution of chemical heterogeneity, which are more easily observed when running long experiments. Chemical differentiation of the models takes place in the initial stage of the numerical experiments by partial melting of a pristine mantle. The numerical model, partial melting, the rheology model, and the experimental setup are described below.

2.1 Model equations

S

Applying the Boussinesq approximation, the following nondimensional expressions for the conservation of momentum, mass, and energy can be derived, in which internal heating is ignored:

$$\partial_j \tau_{ij} - \partial_i \Delta p - (RaT - RbF) = 0, \quad \partial_j u_j = 0 \tag{1}$$

$$\frac{\partial T}{\partial t} + u_j \partial_j T = \partial_j \partial_j T.$$
⁽²⁾

For symbol explanations, see Table 1. The thermal and chemical driving forces of convection are scaled by the thermal and chemical Rayleigh numbers *Ra* and *Rb*, respectively:

$$Ra = \frac{\rho_0 g \alpha \Delta T h^3}{\eta_0 \kappa} \tag{3}$$

Table 1. Symbols of the energy, momentum and continuity eqs (1)-(2).

ymbol	Property	Definition	Unit
В	Viscosity pre-factor		Pa s
c_p	Isobaric heat capacity		$1250 \rm Jkg^{-1} K^{-1}$
e_{ij}	Strain-rate tensor	$\partial_j u_i + \partial_i u_j$	s^{-1}
\overline{F}	Degree of depletion		$\rm kg~kg^{-1}$
g	Acceleration due to gravity		9.81 m s^{-2}
h	Length scale		$670 \times 10^3 \text{ m}$
Δp	Dynamic pressure perturb.	$p - \rho_0 gz$	Ра
\mathcal{Q}	Activation energy		Jmol ⁻¹
t	Time		S
Т	Temperature		K
T_0	Surface temperature		273 K
ΔT	Temperature scale		1775–1850 K
Ζ	Depth		m
α	Thermal expansion coeff.		$3 \times 10^{-5} \mathrm{K}^{-1}$
δρ	Chemical density difference		$\mathrm{kg}\mathrm{m}^{-3}$
$\frac{\partial \rho}{\partial F}$	Chemical density variation		$-226 \text{kg} \text{m}^{-3}$
η	Viscosity		Pa s
η_i	Internal viscosity		Pa s
η_T	Temperature induced		
	viscosity contrast		
η_W	Water induced viscosity		
	contrast		
κ	Thermal diffusivity		$10^{-6} \mathrm{m^2 s^{-1}}$
ρ_0	Reference density		$3416 \text{kg} \text{m}^{-3}$
τ_{ij}	Deviatoric stress tensor	ηe_{ij}	Ра

$$Rb = \frac{\delta\rho h^3}{\eta_0 \kappa} \tag{4}$$

with $\delta \rho$ the density difference at full depletion.

In the numerical experiments, either a uniform viscosity for the entire domain (end-member model) or an Arrhenius type viscosity with an additional pre-factor f(w) prescribing the increase of the viscosity due to dehydration is applied:

$$\eta = f(w)B \exp(Q/RT). \tag{5}$$

The activation energy Q is calculated to correspond to a specified viscosity contrast η_T for the prescribed temperature contrast of the model:

$$Q = \frac{\ln(\eta_T)RT_0(T_0 + \Delta T)}{\Delta T}$$
(6)

$$B = \eta_i \eta_T \exp\left(\frac{-Q}{RT_0}\right). \tag{7}$$

Values for Q range from around 6 kJ mol⁻¹ for $\eta_T = 10$ to about 30 kJ mol⁻¹ for $\eta_T = 10^5$. The pressure dependence of the viscosity (see Karato & Wu 1993) is not considered.

The additional pre-factor f(w) varies linearly between 1 (wet) and a factor η_w (dry) for the local water content. Values up to $\eta_w = 100$ are applied, consistent with experimental studies (Hirth & Kohlstedt 1996).

Partial melting is included by irreversibly evolving a parameter called the *degree of depletion* F, which describes the mass fraction of melt which has been extracted, using Lagrangian particle tracers. F varies linearly with temperature between the solidus and the liquidus at constant pressure, for which the data from Herzberg & Zhang (1996) is used, see De Smet *et al.* (1999). Each time step, the local degree of depletion is adjusted in upward direction to the value corresponding to the local temperature and solidus/liquidus temperatures. The melt is assumed to escape instantaneously to the surface and plays no further role. The depleted residue, however, is central in the following. Compaction of the depleted residue is neglected. This introduces an error which is proportional to the degree of depletion.

Any change in degree of depletion results in the complete removal of water at that location, which affects the viscosity through expression (5). Note that as a result of this, the depletion and water field are not identical, as the composition values are somewhere in the range of 0-1, whereas water contents are either 0 or 1 (although interpolation of tracer values may result in non-binary local values).

2.2 Experimental setup

The numerical experiments are performed in an aspect ratio 1 box with free slip mechanical boundary conditions, a 273 K surface temperature and a temperature of $(273 + \Delta T)$ at the lower boundary. The vertical boundaries are thermally insulated. The computational domain is discretized using 3200 quadratic finite elements for solving the Stokes and continuity eqs (1). The quadratic elements are subdivided in four linear subelements each for the energy eq. (2). 2×10^5 particle tracers are used to evaluate the composition and water fields. Tracers are advected using a fourth order Runge–Kutta scheme. Each tracer carries its own value of any prescribed function (degree of depletion, water content), rather than using the local tracer density or density ratio of two types of tracers as a measure of these properties (Tackley & King 2003). Tracer function values are interpolated to the finite element mesh using a particle-in-cell method (Hockney & Eastwood 1988). Some benchmark and resolution test results of the code are presented in Appendix A.

The numerical experiments are started with a homogeneously undepleted, wet box with a cooled half-space temperature distribution (50–150 Myr). This is perturbed in the lower left corner by 1– 2 per cent to promote the onset of a single convection cell. Conditions matching a range of Rayleigh numbers (based on the internal hydrated viscosity) are prescribed, as are the values of η_T and η_w . Additionally, to vary the amount of melt which is produced, the temperature contrast over the domain and the amplitude of the initial thermal perturbation are varied slightly. As soon as convection has been initiated, partial melting starts to take place in the upwelling limb, resulting in the chemical depletion and dehydration of part of the model domain. Exact conditions are specified in Table 2 for all differentiated models. It is the evolution of these chemically differentiated systems which is studied here.

2.3 Results

2.3.1 Modes of thermochemical convection

Nearly all of the numerical experiments which were performed show both prolongued periods of thermochemical convection in a (near) statistical steady state and transient stages during their evolution (see Table 2). The latter occur at the start of the evolution, and in some numerical experiments also during a change from one near statistical steady state to the next. The convection modes observed during the periods of near statistical steady state can be divided into four different types (see Fig. 1).

(i) A stable chemical lid over the entire width of the domain (Fig. 1a).

(ii) A partial chemical lid (Fig. 1b).

(iii) Depleted material taking part in the domain-wide convection. This can take place in the form of a more or less uniform depleted zone in the outer part of the convection cell (Fig. 1c), as non-uniform depleted material and blobs in the outer part of the convection cell (Fig. 1d), or with the depleted material more or less homogenously distributed throughout the domain (Fig. 1e).

(iv) No chemical differentiation (Fig. 1f).

As can be seen in each of the results presented in Table 2, a (near) statistical steady state can be maintained for very long times (0.15–0.9 h^2/κ).

The occurrence of the different types of dynamics depends mainly on the amount of melting in the initial stage of the runs, which depends on the initial condition and the rheology model. All types have been observed for somewhat overlapping ranges in prescribed parameters. However, for stronger temperature dependence of the viscosity ($\eta_T = 10^3 - 10^5$), experiments which initially had a chemical lid showed continuous transient behaviour towards remixing of the lid during the entire run rather than periods of a near statistical steady state, making them less suitable for the approach applied here.

2.3.2 Semi-empirical scaling law of heat flow

For an isoviscous bottom-heated thermally convective system, the vigour of convection is described by the Rayleigh number (e.g. Turcotte & Schubert 2002):

$$Ra = \frac{\rho_0 g \alpha \Delta T h^3}{\eta \kappa}.$$
(8)

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Table 2. Summary of numerical experiment conditions and results for all differentiated models. *pert.* indicates the perturbation applied to the initial temperature field, which is a cooled half-space of age *ini. ph.* indicates the phase for numerical experiments which show distinct phases of different behaviour. t_{start} and t_{end} are the starting and ending times of the phase, respectively. $\langle Nu \rangle$ and *VRMS* indicate the time average (over the specified period) of the top boundary averaged Nusselt number and rms velocity, respectively. $\langle Nu \rangle$ and *VRMS* indicate the time average (over the specified period. *class* refers to the classification discussed in the text. The characterizations listed under *char*: have the following meanings: **S**—stable depleted zone at entire top boundary; **I**—internal convection/mixing in depleted zone; **E**—erosion of depleted zone; **C**—stable depleted zone in one top corner; **M**—movement of depleted zone along top boundary; **B**—advection of blobs along outer boundary; **Z**—advection of depleted zone along outer boundary and **R**—complete remixing. Classification numbers I, II and III indicate a full chemical lid, a partial chemical lid and depletion advection, respectively. Subclasses 1, 2 and 3 of the latter represent depleted outer zone, more or less fully remixed, and blob advection cases, respectively. Superscript letters refer to frames in Fig. 1.

Ra	ΔT	η_T	η_W	pert.	ini.	ph.	$t_{\rm start}$	tend	$\langle Nu \rangle$	VRMS	$\langle \eta \rangle$	char.	Class
3×10^4	1775	1	1	0.01	150	1	0.6	1.25	4.87	53.28	1	CE	Π^b
3×10^4	1775	1	10	0.02	150	1	0.75	1.45	5.02	44.66	2.74	Ζ	III.1
3×10^{4}	1775	1	100	0.01	150	1	0.6	1.5	4.05	33.85	8.69	В	III.3
3×10^{4}	1775	1	10	0.01	150	1	0.15	1.5	5.11	47.66	2.72	Z	III.1
3×10^4	1775	1	100	0.02	150	1	0.75	1.45	4.04	34.32	8.52	В	III.3
3×10^{4}	1775	10	1	0.01	150	1	0.45	0.75	5.4	56.99	1.46	R	III.2
3×10^4	1775	10	10	0.02	150	1	0.75	1.45	3.47	29.75	3.96	Z	$III.1^{c}$
3×10^{4}	1775	10	100	0.02	150	1	0.5	1.4	2.75	24.57	11.42	В	III.3
3×10^4	1775	10	1	0.01	150	2	0.9	1.2	5.67	62.32	1.45	R	III.2
3×10^{4}	1775	10	10	0.01	150	1	0.5	1.5	3.57	30.85	3.86	Z	III.1
3×10^{4}	1775	10	100	0.01	150	1	0.3	1.5	2.81	25	11.73	В	III.3
3×10^{4}	1800	1	1	0.01	150	1	0.5	1.5	2.52	30.72	1	SI	Ι
3×10^{4}	1800	1	10	0.01	150	1	0.5	1.5	5	44.85	2.95	R	III.2
3×10^{4}	1800	1	100	0.01	150	1	0.3	1.5	4.08	35.67	9.63	В	III.3
3×10^{4}	1800	10	1	0.01	150	1	0.3	0.75	3.6	37.9	1.55	CE	II
3×10^{4}	1800	10	10	0.01	150	1	0.3	1.5	3.28	27.6	4.55	Z	III.1
3×10^{4}	1800	10	100	0.01	150	1	0.3	1.5	2.59	23.11	14.44	В	III.3
3×10^{4}	1800	10	1	0.01	150	2	1	1.5	5.61	61.05	1.46	R	III.2
3×10^{4}	1825	1	10	0.02	150	1	0.75	1.5	4.85	41.48	3.23	R	III.2
3×10^{4}	1825	1	100	0.02	150	1	0.3	1.5	3.86	31.58	11.5	В	III.3
3×10^{4}	1825	10	10	0.02	150	1	0.75	1.5	3.59	27.63	4.61	Z	III.1
3×10^{4}	1825	10	100	0.02	150	1	0.3	1.5	2.53	21.44	18.09	В	III.3
3×10^{4}	1825	100	10	0.02	150	1	0.25	1.5	3.64	39.36	3.55	Z	III.1
3×10^{4}	1850	1	10	0.02	150	1	0.94	1.4	4.5	36.79	3.46	R	III.2
3×10^{4}	1850	1	100	0.02	150	1	0.4	1.2	3.41	26.86	13.52	В	III.3
3×10^{4}	1850	10	100	0.02	150	1	0.25	1.25	2.33	19.43	21.62	В	III.3
3×10^{4}	1850	100	10	0.02	150	1	0.4	0.75	3.29	34.1	4.87	Z	III.1
105	1775	1	1	0.01	50	2	0.4	0.5	7.66	125	1	R	III.2
105	1775	1	1	0.01	150	1	0.05	0.4	2.91	60.57	1	S	Ι
105	1775	1	10	0.01	50	2	0.32	0.5	6.29	70.48	4.22	R	III.2
105	1775	1	10	0.02	150	1	0.28	0.5	6.91	83.4	3.85	R	III.2 ^e
105	1775	1	10	0.01	150	2	0.3	0.5	7.13	86.24	3.96	R	III.2
105	1775	1	100	0.02	150	1	0.2	0.5	4.26	46.95	15.28	В	111.3
105	1775	1	100	0.01	150	1	0.15	0.5	4.09	43.18	15.39	В	111.3
105	1775	10	I	0.01	100	l	0.5	1	3.19	63.02	1.41	SI	I
105	1775	10	1	0.01	50	l	0.3	0.5	3.09	61.57	1.41	S	l
105	1775	10	1	0.01	150	1	0.2	0.5	3.08	61.45	1.41	S	I II A
105	1775	10	10	0.01	150	1	0.28	0.5	5.77	62.44	4.67	R	111.2
105	1775	10	10	0.01	100	1	0.5	1	5.58	60.95	4.8	R	111.2
105	1775	10	10	0.02	150	1	0.35	0.5	5.54	61.23	4.79	R	111.2
105	1775	10	10	0.01	50	1	0.3	0.5	5.58	60.92	4.84	Z	111.1
105	1//5	10	100	0.02	150	1	0.25	0.5	3.96	43.54	19.87	В	111.3
105	1775	10	100	0.01	50	1	0.3	0.5	4.34	48.39	18.15	В	111.3
105	1//5	10	100	0.01	150	1	0.2	0.5	3.96	42.74	19.28	В	111.3
105	1//5	100	1	0.01	150	1	0.05	0.125	3.39	62.75	2.94	В	111.3
105	1775	100	1	0.01	50	1	0.1	0.15	3.73	58.36	2.85	В	111.3
105	1//5	100	1	0.01	50	2	0.3	0.5	6.07	96.65	2.51	K	III.2 III.1
105	1//5	100	1	0.01	150	2	0.27	0.5	5.96	93.43	2.54		
105	1//3	100	10	0.01	150	1	0.15	0.5	3.68	40.03	10.83		111.1 TT 1
105	1/75	100	10	0.02	150	1	0.25	0.5	5.65	44.6	11.26	Z	111.1 TT 1
105	1//3	100	10	0.01	100	1	0.75	1.5	3.52	45.0	11.72		111.1
105	1/75	100	10	0.01	50	1	0.25	0.5	5.69	40.15	10.83	Z	111.1 TT 1
105	1//3	100	100	0.02	150	1	0.5	0.5	3.4Z	30.1/	19.00		111.1
105	1/75	100	100	0.01	150	1	0.1	0.5	5.85	40.66	14.56	В	111.3
105	1775	100	100	0.01	50	1	0.15	0.5	4.21	55.72	11.55	В	111.3

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Table 2. (Table 2. (Continued.)												
Ra	ΔT	η_T	η_W	pert.	ini.	ph.	t _{start}	tend	$\langle Nu \rangle$	VRMS	$\langle \eta \rangle$	char.	Class
10 ⁵	1800	1	10	0.01	150	2	0.35	0.5	7.04	84.32	3.84	R	III.2
10^{5}	1800	1	100	0.01	150	1	0.25	0.5	3.49	35.38	15.29	В	III.3
105	1800	10	1	0.01	150	1	0.15	0.5	2.85	57.63	1.4	S	Ι
10 ⁵	1800	10	10	0.01	150	1	0.15	0.3	3.64	51.15	6.63	CV	II
105	1800	10	10	0.01	100	1	1.1	1.5	5.43	57.95	5.11	R	III.2
105	1800	10	100	0.01	150	1	0.2	0.5	3.68	41.82	22.97	В	III.3
105	1800	100	1	0.01	150	1	0.35	0.5	6.02	94.26	2.5	R	III.2
105	1800	100	10	0.01	150	1	0.2	0.5	3.76	40.96	10.06	Z	
105	1800	100	100	0.01	150	1	0.1	0.5	3.20 4.52	57.92	23.99	В	III.5 II
10 ⁵	1825	1	100	0.02	150	1	0.35	0.5	4.32	38.80	5.65 17.03	7	II III 1
10 ⁵	1825	10	100	0.02	150	1	0.5	0.25	2.32	42.17	6 99	SE	I
10^{5}	1825	10	10	0.02	150	2	0.35	0.5	3.18	47.95	6.85	C	II
10 ⁵	1825	10	100	0.02	150	1	0.2	0.5	3.57	40.99	28.19	В	III.3
10^{5}	1825	100	100	0.02	150	1	0.3	0.5	2.88	32.75	35.54	В	III.3
10 ⁵	1850	1	10	0.02	150	1	0.2	0.5	2.46	41.17	3.81	SE	Ι
10 ⁵	1850	1	100	0.02	150	1	0.2	0.5	4.03	40.64	23.95	В	III.3
10^{5}	1850	100	100	0.02	150	1	0.1	0.5	2.42	31.64	47.46	В	III.3
3×10^5	1775	1	1	0.01	150	1	0.15	0.32	4.35	125.7	1	SI	Ι
3×10^{5}	1775	1	1	0.01	150	2	0.6	0.65	10.01	195.62	1	R	III.2
3×10^{5}	1775	1	10	0.01	150	2	0.4	0.7	8.65	129.82	5.23	R	III.2
3×10^{5}	1775	1	10	0.02	150	1	0.5	0.7	8.48	122.45	5.41	R	III.2
3×10^{5}	1775	1	100	0.02	150	1	0.2	0.65	5.71	64.94	18.18	Z	III.1
3×10^{5}	1775	1	100	0.01	150	1	0.3	0.7	5.55	59.39	18.11	Z	III.1
3×10^{5}	1775	10	1	0.01	150	1	0.15	0.45	3.59	109.3	1.34	SI	I Ia
3×10^{5}	1//5	10	1	0.01	100	2	0.6	0.75	4.24	117.04	1.41	SE	I" I
3×10^{-5}	1775	10	1	0.01	100	1	0.2	0.55	5.04	112.14 94.9	6.0	SE	1
3×10^{5}	1775	10	10	0.01	150	1	0.35	0.45	4.86	04.0 83.25	6.83	CE	11 11
3×10^{5}	1775	10	10	0.01	100	2	0.55	0.75	7.57	110.52	5.66	R	III 2
3×10^{5}	1775	10	10	0.02	150	1	0.33	0.75	4.52	82.04	6.75	CE	II
3×10^{5}	1775	10	100	0.01	150	1	0.25	0.7	3.62	38.27	31.46	Z	III.1
3×10^5	1775	10	100	0.02	150	1	0.33	0.75	3.63	38.41	31.42	Ζ	III.1
3×10^5	1775	100	1	0.01	150	1	0.1	0.2	3.54	100.64	2.61	SE	Ι
3×10^5	1775	100	1	0.01	150	2	0.55	0.7	9.06	198.33	2.25	R	III.2
3×10^{5}	1775	100	10	0.02	150	2	0.52	0.65	5.15	75.66	10.77	R	III.2
3×10^{5}	1775	100	10	0.02	150	1	0.33	0.45	4.52	73.61	14.08	CE	II
3×10^{5}	1775	100	10	0.01	150	1	0.15	0.3	3.76	75.54	15.29	CE	II
3×10^{5}	1775	100	10	0.01	100	1	0.45	0.75	5.39	83.26	10.68	R	III.2
3×10^{5}	1775	100	10	0.01	150	2	0.5	0.6	5.75	87.5	9.2	R	III.2 III.1
3×10^{5}	1//5	100	100	0.02	150	1	0.4	0.65	2.83	41.74	59.59 62.29		
3×10^{5}	1800	100	100	0.01	150	1	0.55	0.7	2.09	43.75	3.88	CE	111.1 11
3×10^{5}	1800	1	100	0.01	150	1	0.15	0.5	5.65	59.01	20.47	7	III 1
3×10^{5}	1800	10	10	0.01	150	1	0.3	0.55	3.5	75.28	6.85	Č	II
3×10^{5}	1800	10	10	0.01	100	1	0.4	0.52	3.49	72.97	6.91	C	II
3×10^5	1800	10	100	0.01	150	1	0.3	0.75	4.43	46.06	29.66	В	III. 3^d
3×10^5	1800	100	1	0.01	150	1	0.3	0.75	3.55	102.64	2.66	SI	Ι
3×10^5	1800	100	10	0.01	150	1	0.15	0.3	2.98	67.92	18.39	CE	II
3×10^{5}	1800	100	10	0.01	100	1	0.52	0.75	4.17	71.32	16.62	CE	II
3×10^{5}	1800	100	10	0.01	150	2	0.5	0.75	4.3	71.19	17	CE	II
3×10^{5}	1800	100	100	0.01	150	1	0.5	0.75	3.07	29.6	61.34	Z	III.1
3×10^{-5}	1825	1	10	0.02	150	1	0.2	0.4	2.93	72.1	3.61	SE	I
3×10^{5}	1825	1	100	0.02	150	1	0.35	0.5	5.69	56.93	23.41	R	111.2
3×10^{5}	1825	10	10	0.02	150	1	0.4	0.75	2.81	08.87	0.85	S	1
3×10^{5}	1825	10	100	0.02	150	1 1	0.21	0.32	3.13 2.17	40.02	55.28 17.93	SE B	111.3 T
$3 \times 10^{\circ}$ 3×10^{5}	1825	100	10	0.02	150	1	0.12	0.28	2.4/	37.96	17.85	SE P	1
3×10^{5}	1850	100	100	0.02	150	1	0.5	0.75	3.33 2.77	69.21	3.68	S	111.2 T
3×10^5	1850	1	100	0.02	150	1	0.5	0.75	4.84	41 97	32 94	R	
3×10^{5}	1850	100	10	0.02	150	1	0.4	0.75	2.62	61.38	20.3	S	III.2
3×10^{5}	1850	100	100	0.02	150	1	0.4	0.75	3.06	27.65	73.79	R	III.2
106	1775	100	1	0.01	100	1	0.08	0.2	3.76	170.93	2.46	SE	Ι
10^{6}	1775	100	10	0.01	100	1	0.07	0.1	2.92	117.63	14.9	SE	Ι



Figure 1. Characteristic snapshots for each of the (sub)types of thermochemical convection which were observed in the set of numerical experiments. The columns show, from left to right, the degree of depletion *F*, the temperature, the water content, the logarithm of the viscosity $log(\eta)$, and time-series of the volume averaged temperature $\langle T \rangle$ (solid), the Nusselt number *Nu* (short-dashed), and the rms velocity *vrms* (long-dashed). The six (sub)types are: (a) full chemical lid, (b) partial chemical lid, outer shell depletion, (d) outer shell depleted blobs, (e) homogeneous depletion and (f) undepleted (purely thermal convection).

A measure of convective heat transport is the Nusselt number, defined as (for a square domain):

$$Nu = \frac{1}{k\Delta T} \int_{x=0}^{l} k \frac{\partial T}{\partial z} dx.$$
(9)

The classical relation between Ra and Nu obtained by Turcotte & Oxburgh (1967) for an isoviscous system is of the form

$$Nu = \lambda Ra^{\beta}.$$
 (10)

The exponent β has a value of $\frac{1}{3}$ and the constant λ is 0.294 (theoretical value) or 0.225 (numerically obtained value, Turcotte & Schubert 2002). For a rheology which is weakly dependent on temperature, these formulations remain applicable (Solomatov 1995). In this work, thermally induced viscosity variations in numerical experiments showing prolongued near statistical steady states are two orders of magnitude or less, and the same goes for water-induced viscosity variations. Convection of highly temperature dependent fluids is treated elsewhere for thermal systems (e.g. Solomatov 1995; Reese *et al.* 1998) and below for thermochemical systems using a different approach.

The relation between Ra and Nu is shown for all chemically differentiated statistical steady states in Fig. 2, which plots the 'effective' Rayleigh number Ra_{eff} on the horizontal axis and the Nusselt number on the vertical axis, both using a logarithmic scale. This effective Rayleigh number uses the domain average viscosity instead of the viscosity scale, incorporating the effects of both temperature and dehydration:

$$Ra_{\rm eff} = \frac{\rho_0 g \alpha \Delta T h^3}{\langle \eta \rangle \kappa}.$$
 (11)

Best fits corresponding to the following expression were calculated:

$$Nu = \lambda Ra_i^\beta \tag{12}$$

with Ra_i either representing the purely thermal Rayleigh number Ra or the 'effective' Rayleigh number Ra_{eff} . The results are listed in Table 3.



Figure 2. Relation between convective vigour $[\log(Ra_{eff}), \text{ see expression} (11)]$ and surface heat flow $[\log (Nu), \text{ see expression (9)}]$. Square symbols indicate results for full lid cases; crosses indicate results for partial lid cases; triangles indicate results for depletion advection cases. The solid lines show least squares fits, listed in Table 3. Dashed lines indicate theorical predictions for purely thermal convection for $\lambda = 0.294$ (theoretical value) and $\lambda = 0.225$ (value based on numerical simulations, Turcotte & Schubert 2002). The inset shows the width *w* of the partial chemical lid for appropriate cases. The circle in this inset shows an outlier which was ignored in the construction of the contour map.

Table 3. Fitting parameters for the Ra - Nu and $Ra_{eff} - Nu$ relations for different dynamic regimes.

Regime		Ra		$Ra_{\rm eff}$					
	N	λ	β	R^2	λ	β	R^2		
Full chemical lid	21	0.99	0.093	0.44	0.47	0.17	0.91		
Partial chemical lid	16	4.13	-0.0036	-0.02	1.86	0.08	0.22		
Remixing	82	1.15	0.12	0.31	0.35	0.27	0.88		

From these results it is clear that the heat transfer characteristics of the system are better described by an average Rayleigh number for the entire domain than for a more specific Rayleigh number which focuses on the main convection cell in the 'mantle', but which does not take the slowly convecting chemical lid into account.

Fig. 2 shows that the results for the depletion advection cases are quite close to those for purely thermal convection. The full chemical lid cases consistently plot on a single trend which has a lower slope of about 0.17. Partial lid results plot in between these trends. The inset of Fig. 2 shows that the behaviour is generally closer to purely thermal convection and depletion advection cases for a smaller width of the chemical lid, as is to be expected.

The effect of the chemical lid is illustrated in Fig. 3, which shows a temperature snapshot for a non-differentiated and a differentiated model with $Ra = 10^6$. Whereas the purely thermal case shows a single whole-domain convection cell, the thermochemical case shows two large convection cells in the mantle underneath the chemical lid, two small-scale convection cells in the bottom part of the chemical lid, and a thermal lid which is much thicker and more irregular than in the purely thermal case. The chemical lid, when thicker than



Figure 3. Temperature field and stylized flow directions for a purely thermal convection case (left) and a thermochemical convection case (right), both for a *thermal* Rayleigh number of 10^6 and $\eta_T = 10^2$. Arrows indicated general directions of flow. The dashed line indicates the base of the chemical lid in the thermochemical case.

the 'natural' thermal lid thickness, greatly affects the thickness of the thermal lid, thus significantly reducing the heat flow out of the system. However, this may be mitigated by convection in the lower part of the chemical lid.

3 SCALING-LAW APPROACH

As shown in the previous section, a significant deviation from classical scaling laws of heat flow can occur when a chemical stratification is present. This specific case, corresponding to the full lid case of Fig. 1(a), is studied in more detail in this section, applying existing scaling laws to stratified scenarios. The system is approximated by several different 1-D scenarios. Fig. 4 shows four (end-member) cases which are discussed below. This approach is also used to determine to which extent the results of the previous section that use a relatively small temperature dependence of the viscosity, are applicable to geologically more relevant rheologies. In this section, results are consistently presented in terms of whole the domain Rayleigh number based on the internal viscosity (expression 8) and the whole domain Nusselt number (expression 9), as would be done when considering a single thermal convection system. However, calculations are based on local Ra and Nu numbers for individual layers, as described below. The solutions presented in Sections 3.2–3.5 are obtained numerically using a bisection algorithm by requiring a constant heat flow through the layers. Heat flow is generally calculated from the Nusselt number:

$$q_i = N u_i k \frac{\delta T_i}{\delta z_i}.$$
(13)

Additional expressions required for finding solutions are:

$$\delta T_1 + \delta T_2 = \Delta T \tag{14}$$

and

$$\delta z_1 + \delta z_2 = h. \tag{15}$$

3.1 Single-layer thermal convection

The basic model to which all layered models are to be compared is the classical single-layer model. The surface heat flow for this model is plotted in Fig. 5, for isoviscous cases (a), and for temperature and strain-rate dependent rheologies for two different stagnant lid models, flat roof (b and c) and large lid slope (d and e), which will be discussed below. Fig. 5(a) is based on eqs (8)–(9), Figs 5(b)–(e) are based on equations by Reese *et al.* (1998) which are discussed in Section 3.5.



Figure 4. Four end-member scenarios for the thermal structure of a chemical lid and underlying convecting mantle. (a) internally immobile chemical lid, (b) convection in entire chemical lid, (c) top part of lid is conductive, bottom part of lid is convecting and (d) as (c) with a single scaling law for the convecting and conducting part of the chemical lid.



Figure 5. log(Ra) - log(Nu) relations for (a) isoviscous models (Turcotte & Schubert 2002), (b and c) flat roof stagnant lid models (Reese *et al.* 1998) with strain-rate exponent n = 1 and 3 and (d and e) large slope stagnant lid models (Reese *et al.* 1998) with n = 1 and 3. The activation energy Q of the temperature dependent rheology is indicated on the horizontal axis in the latter two cases.

3.2 Conducting chemical lid

When a chemical lid is completely internally immobile, and when it is sufficiently thick, the system can be approximated as a conductive layer on top of a isoviscous convecting layer, as shown in Fig. 4(a). The heat flow of the conducting top layer can be described directly:

$$q_1 = k \frac{\delta T_1}{\delta z_1} \tag{16}$$

and that of the convecting bottom layer by

$$Nu_i = \lambda Ra_i^\beta \tag{17}$$

with

$$Ra_i = \frac{\rho g \alpha \delta T_i \delta z_i^3}{\eta_i \kappa}.$$
(18)

By demanding that $q_1 = q_2$, obtaining q_2 from expressions (13), (17) and (18), the temperature T_1 and thus the surface heat flow can be determined as a function of z_1 . Fig. 6 shows the surface heat flow [as log(Nu)] as a function of chemical lid thickness z_1 and the Rayleigh number Ra defined for the entire system. As Ra increases, the temperature contrast across the lid approaches ΔT , which corresponds to the maximum possible heat flow for this configuration.

3.3 Fully convecting chemical lid

In the second case, shown in Fig. 4(b), the chemical lid is fully convecting. In this simplification, a uniform viscosity for each of the two layers is assumed, but they are not necessarily equal.



Figure 6. Logarithmic Nusselt number as a function of chemical lid thickness and whole domain Rayleigh number Ra for the immobile lid case (Fig. 4a).

As in this scenario the interface temperature (free parameter) is not a function of the layer thickness but only of the viscosity contrast between the layers, it can be easily shown that the heat flow is not a function of the depth of the interface.

$$Ra_1 \sim z_1^3, \ Ra_1 \sim T_1 \tag{19}$$

$$Nu_1 \sim Ra_1^{1/3}$$
 (20)

$$q \sim Nu/z_1, \ q \sim T_1^{1/3}.$$
 (21)

Again the heat flow of the two layers, described by eqs (17) and (18), is demanded to be equal. The resulting surface heat flow is shown in Fig. 7 (logarithmic), where the shaded area indicates conditions which do not allow convection (i.e. which have local Rayleigh numbers below the critical Rayleigh number $Ra_{crit} = 657.5$, Turcotte & Schubert 2002). Note that the Rayleigh number on the vertical axis is based on the viscosity of the lower layer. Increasing the whole domain Rayleigh number results in an increase of the heat flow. The lower limit *Ra* for convection to take place increases with increasing viscosity of the top layer.

3.4 Convecting chemical lid bottom

More realistic than the previous case is the third, which has a conductive upper chemical lid, and a convecting lower chemical lid on top of a convecting mantle (see Fig. 4c).

The heat flow of each convecting layer can be expressed as a Nusselt number using expression (17). The conductive lid is described by eq. (16). By equating the heat flow of all three layers, the interface temperatures T_1 and T_2 can be determined as a function of the interface depths z_1 and z_2 and thus the heat flow of the system.

Fig. 8 shows the surface heat flow, expressed as the logarithmic Nusselt number, for this scenario, for several different values of the chemical lid thickness and the viscosity ratio of the two convecting layers. For low whole domain Rayleigh numbers, no convection takes place, and the lower limit increases with increasing viscosity of the bottom part of the chemical lid. For increasing Rayleigh numbers, the heat flow is determined more and more by the thickness of the conductive lid.

3.5 Stagnant lid scaling of chemical lid

The whole of the chemical lid can be approached from a stagnant lid scaling law perspective (Fig. 4d). Reese et al. (1998) describe two end-member modes of operation for the stagnant lid regime. The first is the large lid slope mode, in which the slope of the base of the lid is steep, and shear stresses in the thermal boundary layer are large. The second is the *flat roof* mode, which has a small inclination of the lid base and smaller shear stresses in the boundary layer. There are no theoretical constraints on the slope of the base of the lid (Reese et al. 1998). Results for full lid cases in Section 2 show an increasing slope for increasing lid thickness and decreasing Rayleigh number, ranging from about 10° for $\log(Ra_{\text{eff}}) = 5.0-5.5$ and $d_{\text{lid}} = 0.15-0.2$ to around 30° for $\log(Ra_{eff}) = 4.0-4.5$ and $d_{lid} = 0.25-0.3$. The aspect ratio of the box and chemical stratification within the lid will probably also play a role, but the present experiments do not constrain this. Following Reese et al. (1998), the heat flow of the chemical lid, of which the lower part is assumed to be convecting and the upper part the thermal stagnant lid for Newtonian (n = 1)or non-Newtonian (n > 1) deformation, can be described for a flat roof stagnant lid by:

$$Nu_1 = (1.73)^{3(n+1)/(2n+3)} \frac{Ra_n^{n/(2n+3)}}{\theta^{3(n+1)/(2n+3)}}$$
(22)

and for a large lid slope stagnant lid by:

$$Nu_1 = (0.88 + 1.15n) \frac{Ra_n^{n/(2n+3)}}{\theta}$$
(23)



Figure 7. Logarithmic Nusselt number as a function of chemical lid thickness z_1 and whole domain Rayleigh number Ra for the full lid convection case (Fig. 4b). The shaded region indicates conditions where the Ra_1 is smaller than the critical Rayleigh number ($Ra_{crit} = 657.5$), and thus no convection takes place. (a) $\eta_1/\eta_2 = 1$, (b) $\eta_1/\eta_2 = 10$, (c) $\eta_1/\eta_2 = 100$ and (d) $\eta_1/\eta_2 = 1000$.

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Figure 8. Logarithmic Nusselt number as a function of *conductive* lid thickness z_1 and whole domain Rayleigh number Ra for the lid bottom convection case (Fig. 4c). Results are shown for a range of chemical lid thicknesses ($z_2 = 0.2-0.5$) and viscosity ratios ($\eta_2/\eta_3 = 1-1000$). The shaded region indicates conditions where the Ra_1 is smaller than the critical Rayleigh number, and thus no convection takes place, or where $z_1 > z_2$.

with

$$Ra_{n} = \frac{\rho g \alpha \delta T_{1} \delta z_{1}^{(n+2)/n}}{\kappa^{1/n} b^{1/n} \exp(-\gamma T_{i}/n)}.$$
(24)

In the latter expression, the internal temperature T_i of the convecting bottom part of the chemical lid is assumed to be close to the temperature at the bottom of the chemical lid T_1 , allowing us to use T_1 instead of T_i . This approach uses the Frank–Kamenetskii approximation of an Arrhenius viscosity, discussed in Solomatov & Moresi (1996) and Reese *et al.* (1998). The relevant rheological parameters present in expressions (22)–(24) are

$$\gamma = Q/RT_i^2 \tag{25}$$

and

$$\theta = \gamma \Delta T_i \tag{26}$$

with ΔT_i the temperature drop over the thermal lid, Q the activation energy, and R the gas constant. In the scenario of Fig. 4(d), we can expect the temperature contrast over the chemical lid to be very much larger than that over the bottom convecting layer. This is confirmed by numerical experiments which will be discussed below. Therefore, for simplicity $\Delta T_i = \Delta T$ is assumed. This also allows the assumption that temperature and, therefore, viscosity variations in the convecting mantle underneath the chemical lid are minor, which is why it can be approached as an isoviscous layer. By requiring that the stagnant lid heat flow of expression (22) or (23) is equal to the heat flow of the convecting mantle, described by (17), the Nusselt number as a function of whole domain Rayleigh number Ra (based on the mantle viscosity), chemical lid thickness, and rheological parameters can be obtained. The results are shown in Figs 9 and 10, for six different values of the activation energy Qranging from 250 to 500 kJ mol⁻¹ for n = 1 and 3. The contours indicate the logarithm of the whole-domain Nusselt number. The shaded areas show conditions which do not allow convection to take place (predicted local Nusselt number of the upper layer drops below 1). This model predicts that for geologically relevant values of the activation energy Q, convection in the bottom part of the chemical lid can only take place for high whole domain Rayleigh numbers (of the order of 10⁷-10⁸ and higher) for a Newtonian rheology. For a non-Newtonian rheology with n = 3, however, very little is required to initiate convection in the lower part of the chemical lid, starting at Rayleigh numbers of around $10^5 - 10^6$.



Figure 9. Logarithmic Nusselt number as a function of *chemical* lid thickness z_1 and whole domain Rayleigh number Ra for the stagnant lid scaling case (Fig. 4d), assuming a flat roof stagnant lid (eq. 22). Six different values of the activation energy Q are applied, in characteristic ranges for diffusion creep (n = 1) and dislocation creep (n = 3). The shaded region indicates conditions where the predicted Nusselt number for the layer is smaller than 1, and thus no convection will take place.



Figure 10. Same as Fig. 9, but for a large lid slope scaling law (eq. 23) instead of a flat roof scaling law (see Reese et al. 1998).

Part of the stability of continental roots is ascribed to their dryness relative to the mantle, which results in an increase of the viscosity by up to two orders of magnitude (Karato 1986; Hirth & Kohlstedt 1996). Fig. 11 illustrates the effect of such a viscosity increase on the heat flow characteristics of the system for the flat roof and large lid slope formulations, respectively, by showing the migration in parameter space of the boundary of the onset of convection in the lid. In each frame, the pre-factor in the Arrhenius viscosity formulation has been multiplied by an additional factor η_w of 10 or 100 in the uppermost two curves. This results in a shift of the boundary (and also of the Nusselt number isolines which are not shown) towards higher Rayleigh numbers relative to the case with no viscosity increase due to dehydration (lowermost curve in each frame). However, for non-Newtonian cases the shift is significantly less than for Newtonian cases. This results from the $b^{1/n}$ term in the Rayleigh number, expression (24).

4 STRATIFIED NUMERICAL CONVECTION EXPERIMENTS

In this section, the predictions of the convecting lid model of Section 3.5 with temperature and strain-rate dependent rheology are tested using a series of numerical experiments.



Figure 11. Boundary of the convecting region as a function of *chemical* lid thickness z_1 and whole domain Rayleigh number Ra for a flat roof (FR) and large lid slope (LLS) stagnant lid cases, for three different values of the dehydration viscosity factor ($\eta_w = 1$, 10, 100). The lowermost curves correspond to the edges of the shaded area the middle frames of Figs 9 and 10. The curves above these correspond to equivalent models with $\eta_w = 10$ and 100, respectively.

4.1 Experimental setup

The numerical experiments are done using the same code as the thermochemical experiments above, using the equations of Section 2.1, but disregarding the compositional terms. This is possible since two-layer convection is explicitly prescribed, and not resulting from density differences. Neglecting the density difference of no more than a few percent in the Rayleigh number results in an error in Raof the same magnitude, and of less than 1 per cent in the predicted heat flow. In these numerical experiments about 1750 quadratic elements are used for solving the Stokes and continuity equations, and four times as many linear elements for the energy equation. The rheology is described by

$$\eta = B \exp\left[\frac{Q}{RT}\right] \tau^{1-n},\tag{27}$$

in which *B* is a pre-factor and τ is the second invariant of the deviatoric stress tensor.

The square domain is divided in two portions that are separated by an impermeable boundary, but which are thermally coupled, that is, temperature is continuous across this boundary. The upper compartment is thought to represent a chemically depleted layer or lid, for example, a continental root, as observed in Fig. 1(a). The lowermost compartment represents the undepleted convecting mantle. The boundary between the two compartments is always horizontal, but its depth is varied for different experiments. Cases with and without mechanical coupling between the two compartments (horizontal velocity is continuous over the internal boundary, and free slip internal boundary, respectively) are investigated. All other boundaries are free slip, and the boxes are heated from below.

4.2 Results

Fig. 12 shows the results of these numerical experiments in terms of convection of the lower part of the top layer representing the chemical lid. Squares indicate convection taking place in the lower part of the top layer, visually perturbing the temperature field. Circles indicate the absence of convection here, and the shaded areas coincide with those of Figs 9 and 10, with the boundaries indicated by solid curves. The results are relatively close to the expected positions in $z_1 - \log(Ra)$ -space. They are, however, not exactly coinciding. Note that no appropriate critical Rayleigh number is considered, but rather the predicted Nusselt number instead, using Nu = 1 as a cut-off value. Davaille (1999) notes that there actually is no critical Rayleigh number for cases like these where there is a horizontal temperature gradient at the boundary. Nevertheless, the results show that the scaling law approach of Section 3.5 predicts convection of the chemical lid quite well. Models with and without mechanical coupling between the upper and lower layer are presented. Obviously models with coupling are more realistic, but the cases without coupling are conceptually closer to the 1-D scaling law setup of



Figure 12. Results of a series of idealized experiments described in Section 4 in terms of convection of the chemical lid. Convection resulting in visible modification of the temperature field relative to a conductive case is indicated by squares. Circles indicate absence of convection. Labels indicate whether mechanical coupling between the layers was used or not (c, nc) and the activation energy in kJ mol⁻¹. The shaded areas indicate where the heat flow scaling law predicts a Nusselt number below 1, so no convection is taking place here. Contours indicate the boundary of this region for the flat roof and large lid slope cases.



Figure 13. Final snapshots of the temperature and flow field and time-series of the Nusselt number of selected numerical layered convection experiments showing convection in the top layer. Characteristics of the individual runs are listed in Table 5.

Section 3.5 and Fig. 4(d). In most numerical experiments, the different approaches result in qualitatively identical results.

To illustrate, Fig. 13 shows snapshots of the temperature and flow field and a Nu number time-series for selected numerical experiments with a convecting lower chemical lid.

5 QUANTITATIVE COMPARISON OF RESULTS

5.1 Numerical thermochemical experiments and scaling law approach

Table 4 lists all thermochemical numerical experiments which have shown a statistical steady state in the full chemical lid mode, together with the corresponding average Nusselt numbers. Also listed is the thickness of the chemical lid, which is used to predict the Nusselt number applying the approaches of Figs 4(a) and (c). For the three layer approach (4c), the conductive lid is assumed to have a thickness of 1/10 of the total chemical lid thickness (a larger

© 2007 The Author, *GJI* Journal compilation © 2007 RAS fraction results in predicting no convection for any of the cases). Only results for $\eta_2/\eta_3 = 1$ are shown, as for higher values, no convection is predicted. Results for the two convecting layer model of Fig. 4(b) are not shown as predictions deviate from observations by 70 per cent or more in all cases. Numerical experiments have been applied to verify the correctness of this model, and though the numerical results also show a deviation in the same direction, it is much smaller, on the order of 20 per cent. The stagnant lid scaling law approach (Fig. 4d) is not applied as it is not suitable for the small temperature dependence of the rheology of these experiments. Predicted values of the Nusselt number are listed together with their relative deviation from the observed value. Best matches are indicated in boldface numbers, and dashes indicate cases where no convection is predicted, which invalidates the model for these conditions. In most thermochemical experiments covering the entire range of Rayleigh numbers, best matches are found for the fully conductive lid model (case a), with deviations of around or less than 10 per cent in most cases. Two cases with a moderate Rayleigh number of 3×10^5 and a relatively low temperature and water dependence of the viscosity show a better match for the three layer model. In

Table 4. Full chemical lid results for the set of differentiated experiments, with fit parameters to the models (a) and (c) of Fig. 4. Dashes indicate conditions for which the respective models predict no convection to take place. Bold-faced entries indicate least difference between the observed and predicted Nusselt numbers. ϵ indicated the relative difference between the predicted and the observed Nusselt numbers ($\epsilon = \lfloor \frac{Nupred - Nuobs}{Nu_{obs}} \rfloor$).

Prescribe	d		Result	s	Model	fits		
Ra	η_T	η_W	Nu	zint	(a)	ϵ	(c)	ϵ
3×10^4	1	1	2.52	0.31	2.14	0.15	_	_
10^{5}	1	1	2.91	0.24	2.86	0.02	_	_
10^{5}	1	10	2.46	0.23	2.96	0.20	_	_
10^{5}	10	1	3.08	0.25	2.82	0.09	_	_
10^{5}	10	1	2.85	0.26	2.71	0.05	_	_
10^{5}	10	1	3.19	0.25	2.82	0.12	_	_
10^{5}	10	1	3.09	0.25	2.82	0.09	_	_
10^{5}	10	10	2.32	0.27	2.59	0.12	_	_
3×10^5	1	1	4.35	0.25	3.02	0.31	4.84	0.11
3×10^5	1	10	2.93	0.23	3.21	0.10	_	_
3×10^5	1	10	2.77	0.24	3.11	0.12	_	_
3×10^5	10	1	4.24	0.26	2.96	0.30	4.79	0.13
3×10^5	10	1	3.64	0.23	3.27	0.10	_	_
3×10^5	10	1	3.59	0.24	3.10	0.14	_	_
3×10^5	10	10	2.81	0.23	3.20	0.14	_	_
3×10^5	100	1	3.54	0.16	4.29	0.21	_	_
3×10^5	100	1	3.55	0.25	2.98	0.16	4.81	0.35
3×10^5	100	10	2.62	0.26	2.96	0.13	4.79	0.83
3×10^5	100	10	2.47	0.28	2.73	0.10	4.61	0.87
10^{6}	100	1	3.76	0.21	3.79	0.01	6.65	0.77
10^{6}	100	10	2.92	0.20	3.90	0.34	6.74	1.31

these cases, the conductive lid model significantly underestimates the heat flow.

5.2 Layered thermal numerical experiments and scaling law approach

A quantitative comparison of the results of the numerical experiments of Section 4 to predictions based on Section 3.5 is presented in Table 5. In most cases, the difference between the numerical experiment and the corresponding theoretical prediction is less than 15 per cent, either for the flat roof model or for the large lid slope model. The latter of these shows a better fit in most cases.

6 DISCUSSION

6.1 Comparison thermal and thermochemical convection

The first set of experiments has shown that, at least for a weakly temperature dependent rheology, depleted material can either be involved the whole-domain convection cycle, in which case it does not significantly affect the system's heat flow characteristics, or it can form a more or less stable stratification, with a light, depleted chemical lid overlying a denser, undepleted or less depleted mantle. In the latter case, again two things can happen, as shown by the thermochemical convection experiments presented in this paper and confirmed for more realistic rheologies in the scaling law approach and layered numerical thermal convection experiments. If the Rayleigh number is sufficiently low, the chemical lid is immobile, also internally, thus providing purely conductive heat transport. In this case, the thickness of the thermal lid is at least equal to the thickness of the chemical lid. For a sufficiently thick chemical lid, this significantly reduces the surface heat flow. If, on the other hand, the Rayleigh number is sufficiently high to allow convection to take place in the lower part of the chemical lid, the heat flow of the system is much closer to a purely thermally convecting system without chemical stratification.

Fig. 14 shows the ratio of the whole domain Nusselt numbers of convecting chemical lid cases to those of conducting chemical lid cases. The regions above the 1-contour, corresponding the limit of convection in the lower chemical lid, show a severalfold increase in the Nusselt number compared to the conducting case, illustrating the efficiency of heat transport in a partly convecting chemical lid.

A comparison of chemically stratified and non-stratified models is made in Fig. 15, which plots the whole domain Nusselt number

Table 5. Heat-flow results for layered convection models with convection in the top layer, with (c) and without (nc) mechanical coupling between the layers. The results are compared to predictions using the flat roof model and the large lid slope model of Section 3.5, showing deviations relative to the observed value. Nusselt numbers refer to whole domain values. ϵ is the relative deviation of the Nusselt number ($\epsilon = |\frac{Nu_{\text{pred}} - Nu_{\text{obs}}}{Nu_{\text{obs}}}|$). Figure references refer to snapshots of temperature and flow field as well as a time-series of the Nusselt number of the respective runs. Reasonable fits ($\epsilon \le 0.15$) are indicated in bold-faced type.

Nume	erical co	nvection n	nodel		Flat roo	of model	Large lid			
Coupling	п	z ₁	Ra	$Q (\mathrm{kJ} \mathrm{mol}^{-1})$	Nuobs	Nupred	ϵ	Nupred	e	Figure
nc	1	0.3	10^{8}	250	5.37	4.87	0.09	7.47	0.39	13a
nc	1	0.3	10^{8}	400	4.28	_	_	4.71	0.10	
nc	1	0.4	10^{8}	250	6.00	4.43	0.26	6.84	0.14	13b
nc	1	0.4	10^{8}	400	4.53	2.58	0.43	4.31	0.05	
nc	1	0.5	10^{7}	250	2.64	2.46	0.07	3.75	0.42	
nc	1	0.5	10^{8}	250	5.98	4.12	0.31	6.38	0.07	
nc	1	0.5	10^{8}	400	4.58	2.39	0.48	4.02	0.12	13c
nc	3	0.2	10^{6}	250	15.5	6.39	0.59	13.1	0.15	
nc	3	0.2	10^{6}	400	10.8	3.91	0.64	9.41	0.13	
nc	3	0.4	10^{6}	250	17.6	5.34	0.70	11.6	0.34	
nc	3	0.4	10^{7}	250	28.8	11.5	0.60	25.1	0.13	
nc	3	0.4	107	400	24.6	6.93	0.72	17.7	0.28	
с	1	0.4	10^{8}	250	4.96	4.43	0.11	6.84	0.38	
с	1	0.4	10^{8}	400	3.52	2.58	0.27	4.31	0.23	
с	3	0.2	10^{6}	400	9.5	3.91	0.59	9.41	0.01	13d
с	3	0.2	10^{7}	400	27.3	8.43	0.69	20.27	0.26	



Figure 14. Ratio of the whole domain Nusselt number for convecting lid cases of Figs 9 and 10 to the conductive chemical lid model of Fig. 4. FR and LLS indicate flat roof and large lid slope, respectively. 250 and 400 indicate the activation energy in kJ mol⁻¹.



Figure 15. Ratio of the whole domain Nusselt number for convecting lid cases of Figs 9 and 10 (above the solid line) and conductive chemical lid cases of Fig. 6 (below the solid line) of a chemically stratified system to the single-layer thermal stagnant lid models of Figs 5(b)–(e). Shaded areas indicate regions where the stratified model has a higher heat flow than the corresponding unstratified model and the model breaks down, see text. FR and LLS indicate flat roof and large lid slope, respectively. 250 and 400 indicate the activation energy in kJ mol⁻¹.

ratio of the former to the latter. Below the solid line, the chemical lid is immobile, as in Figs 4(a) and 6. Above the solid line, part of the chemical lid is convecting. This situation corresponds to Figs 4(d), 9 and 10. Shaded areas show regions where the predicted heat flow of the stratified system is higher than that of its uniform equivalent. This indicates where the model breaks down. This means that the stagnant lid in the purely thermal case is thicker than the immobile or convecting chemical lid. The assumption that the viscosity in the underlying mantle is uniform is no longer valid, and the system behaves as an unstratified one. In the unshaded regions, which coincide with the regions of interest discussed below for the non-linear cases, however, the models hold and a reduction of the heat flow relative to the unstratified case is observed. Below the solid line, that is, for a non-convecting chemical lid, a reduction of a factor 2-5, depending on the conditions, is predicted. Above the solid line, for a partly convecting chemical lid, the reduction in heat flow may be of the same order of magnitude. While in numbers this appears to be relatively minor, it can mean a great deal for the integrated thermal evolution of planets.

The effect of dehydration due to partial melting can be easily included in an effective Rayleigh number as described by expression (11) for weakly temperature dependent rheologies, as is shown in the first part of this work. In general, Figs 7 and 8 show that for a viscosity increase of a factor 200 due to dehydration (Hirth & Kohlstedt 1996), the whole domain Rayleigh number for which convection starts in the bottom part of the lid increases by an order of magnitude. For strongly temperature dependent rheologies, this difference is significant for Newtonian rheology, but smaller for non-Newtonian behaviour with n = 3, as shown by Fig. 11.

6.2 Stability of chemical stratification

In this work, the chemical stratification (undepleted mantle, depleted lid) is shown to be stable for long periods of time for weakly temperature dependent rheologies in the first part. For more realistic rheologies, this stability is assumed in the second part, which requires a justification and discussion.

A theoretical analysis of the problem of convection in immiscible layered systems was presented by Richter & Johnson (1974) for isoviscous systems. Their results are presented only at the low Rayleigh number end of our spectrum, but they suggest that the density contrasts applied in the present study are sufficient to allow separate convection in the two chemically distinct layers in case of an *isoviscous* rheology.

Zaranek & Parmentier (2004) studied the stability and mixing of initially chemically stratified system using numerical experiments with a realistic temperature dependent rheology. It is important to point out here that their experimental setup differs from that presented in this paper in the nature of the composition profile; they apply a linearly varying composition from the top to either the bottom or a specified depth level in the domain, whereas in the present setup, the chemical stratification resembles (first part, see Fig. 1a) or is assumed to be (second part) a step function. The results of Zaranek & Parmentier (2004) show a rapid increase of the onset time for mixing and a rapid decrease of the mixing rate for increasing compositional gradient with depth, and also for increasing activation energy of the rheology (their Fig. 14). More quantitatively, for an internal viscosity of 10¹⁹ Pa s, the initiation time rises to about 600 Myr for an activation energy of 250 kJ mol⁻¹ for a compositional gradient of 0.025 per cent per km. As the lower boundary of the chemical lid in the present experiments is relatively sharp, that is, has a very high gradient, the same effect may be expected to stabilize the lid here. It should however be stressed that the settings are not identical, and that the small depth interval over which the strong compositional gradient is present in the present study corresponds to a much smaller viscosity change over this interval than in the paper of Zaranek & Parmentier (2004). Therefore, the dynamics of the system are not necessarily identical.

Davaille (1999) presented an experimental study of miscible twolayer convection. She used water which was salted to control the density and to which natrosol was added to control the viscosity of each layer. In the range of conditions which she studied $(Ra = 300-3 \times 10^7, \delta\rho/\rho = 0.0045-0.05)$, a two-layer convection system always evolved to a single convecting layer system through penetrative convection. However, the onset time of entrainment of material from one layer into the other was reported to be much longer than the onset time of thermal convection within a layer, as it requires the full development of convection in at least one of the layers (Davaille 1999). More importantly, mixing of one layer into the other may be slow. Using Davaille's analytical analysis, the rate of laminar entrainment of a more viscous upper layer into a less viscous lower layer of equal thickness can be computed:

$$\Phi \approx \kappa L \frac{\alpha \rho \Delta T_B}{\delta \rho} R a_B^{1/5} \tag{28}$$

with the boundary Rayleigh number

$$Ra_B = \frac{\rho \alpha g \Delta T_B L^3}{\eta \kappa}$$
(29)

with the layer thickness L (in a box of dimensions $2L \times 2L \times 2L$), the density difference $\delta \rho$, and the horizontal temperature difference over the interface ΔT_B . Following Davaille (1999), ΔT_B is assumed to be equal to the vertical temperature contrast over the bottom layer. Mixing by plume-shaped upwelling of the lower layer into the upper layer is neglected as it is expected to be less important.

Neglecting the change in the rate of entrainment as the upper layer is 'consumed', the remixing time for the entire layer is

$$\tau_{\rm mix} = \frac{4L^3}{\Phi}.$$
(30)

Fig. 16 shows a contour plot of the remixing time τ_{mix} as a function of depleted layer thickness and whole domain Rayleigh number, for two different values of the chemical density contrast (0.5 and 5 per cent). *flat* and *lls* correspond to the flat roof and large lid slope regimes, respectively. The numbers 3000 and 670 indicate whether a scaling has been performed to a 3000 km deep entire mantle or a 670 km deep upper mantle only. The latter case may be representative of the Archean mantle, as higher mantle temperatures promote layering of convection at a phase transition (Christensen & Yuen 1985). The contours show a kink at the boundary between a convecting and a non-convecting lid. This corresponds to the boundary of the shaded area in Figs 9 and 10 for corresponding rheological parameters.

Strictly speaking, it is incorrect to apply the entrainment rate expression of Davaille to the models presented in Figs 9 and 10, as these have no viscosity contrast over the chemical interface, whereas Davaille assumes a contrast to be present in her derivation. The main effect of this contrast is that material is entrained into the lower layer in the form of sheets, whereas it is entrained into the upper layer in the form of plumes (Davaille 1999). If one assumes entrainment of the upper layer into the lower layer to be laminar even in cases with no viscosity contrast over the interface, the results hold. In this case, Fig. 16 shows that remixing times on the order of less than 100 Myr up to times longer than the age of the Earth are found for varying rheological parameter values and chemical density contrasts between the layers.

From an observational point of view, the roots of cratons are thought to consist of depleted peridotite and they are thought to have survived for billions of years (e.g. King 2005). Numerical models suggest that these roots may be particularly sensitive to erosion by subducting slabs (Lenardic *et al.* 2003), suggesting that chemical lid stability may be more of a problem on Earth than on Mars or Venus.

Overall these works suggest that although erosion of the chemical lid is to be expected, its timescale may be comparable to significantly longer than the characteristic thermal timescale of the lithosphere, which is of the order of 10^8-10^9 yr.

6.3 Application to the terrestrial planets

Before applying the results to the terrestrial planets, first some limitations of the approach should be considered. The scaling laws applied in this work are valid for steady state situations, in which the heat flow through the bottom equals the heat flow through the top of the domain. This observation is also valid for the thermochemical convection simulations of Section 2.3. Although this setup is often applied in studies of the thermal evolution of planets, secular cooling requires that this is not true, that is, more heat is evacuated through the top boundary. In an evolving planet, the balance between these two parameters may constantly shift. Additionally, this work does not consider the effect of internal heating, which may be a source of energy for the upwelling limb of the convection. The effects of cooling from above and internal heating have been studied by Davaille & Jaupart (1993) and Grasset & Parmentier (1998), respectively.

The activation energy of diffusion creep (Newtonian, n = 1), is 240 kJ mol⁻¹ for wet olivine and 300 kJ mol⁻¹ for dry olivine (Karato & Wu 1993). For non-Newtonian dislocation creep (n =3-3.5), Karato & Wu (1993) report values of the activation energy Q of 430 and 540 kJ mol⁻¹ for wet and dry olivine, respectively. If we consider the depth of the interface between the chemical lid and underlying mantle to correspond to the base of the continental roots on Earth (up to some hundreds of km, e.g. Doin et al. 1996; Forte & Perry 2000; King 2005, for a discussion), z_1 would be around 0.15– 0.40 if the upper mantle is considered to convect separately from the lower mantle. For an upper mantle Rayleigh number of the order of 10⁶, Figs 9 and 10 predict no convection in the bottom part of the chemical lid for either case when diffusion creep is assumed to be the main deformation mechanism. When assuming that dislocation creep is dominant, these figures show that only the large lid slope model of Fig. 10 allows convection to take place in the lower parts of the chemical lid. Evidence from both petrological studies (Karato & Wu 1993) and numerical models (Van Thienen et al. 2003) suggests that it is dislocation creep may be important in the shallow mantle and the continental root zone.

Considering the upper mantle may be representative of the early Earth, when convection was more likely to be completely layered (Christensen & Yuen 1985), but not of the present-day situation. When using the entire mantle depth, z_1 ranges from 0.03 to 0.08, and the mantle Rayleigh number is probably of the order of 10^{7} – 10^{8} . In this case, Figs 9 and 10 predict that some convection may take place in the bottom of the lid when the lid is sufficiently thick specifically for the large lid slope case, but again this requires the operation of non-linear rheology.



Figure 16. Logarithm of the remixing time τ_{mix} (in yr) of a more viscous upper layer into a less viscous lower layer of equal thickness by laminar entrainment, following Davaille (1999). The frames coincide with several in Figs 9 (flat roof) and 10 (large lid slope), scaled to the Earth for upper mantle (670) and whole mantle (3000) convection. Two different chemical density contrasts are applied.

Some petrological evidence consistent with convective motion in continental roots was presented by Drury et al. (2001) and Spengler et al. (2006). Drury et al. (2001) present complex reconstructed P,Tpaths for rocks of Precambrian age originating from the Kaapvaal craton. They compare them to numerical models of convective upwelling in the continental root and conclude that diapirism in the continental root is capable of producing these P,T-paths. Spengler et al. (2006) present a geochemical work on Precambrian orogenic peridotites from Norway. They present two models for the P,T-history of these rocks. The first of these, which is their preferred model (Martyn Drury, personal communication 2006), shows the rocks staying at a depth of about 150 km and above the closure temperature of the Sm-Nd isotope system for more than a billion years. For reasonable cooling rates, the closure temperature of this system is between 1000 and 1300 °C (Van Orman et al. 2002). At these temperatures and a pressure of 5 GPa, dry olivine viscosities are of the order 10^{21} - 10^{24} Pa s for diffusion creep and of the order 10^{20} – 10^{22} Pa s for dislocation creep at a strain rate of $10^{-14} \, \text{s}^{-1}$ (Karato & Wu 1993). Thus the material may be quite weak and capable of flowing.



Figure 17. The rms velocity time-series for the code used in this paper (PvT) applied to the thermochemical benchmark of Van Keken *et al.* (1997). For comparison, the results presented in Fig. 12a of Van Keken *et al.* (1997) have been included. Labels PvK, CND, SK, HS and CND Markerchain refer to that figure, see Van Keken *et al.* (1997) for details.



Figure 18. Comparison of snapshots of the temperature and composition and time-series of the Nusselt number and rms velocity for normal resolution experiments (left, black curves) and high resolution experiments (right, grey curves; resolution multiplied by 1.5 in both directions).

As Venus' size is similar to that of the Earth, we can apply the same reasoning to show that convection may be possible in the lower parts of a hypothetical chemical lid. Parmentier & Hess (1992) considered episodic delamination of part of the depleted zone to explain episodic volcanism on this planet. If the lower part of the lid is convecting, this may prevent the build-up of sufficient negative buoyancy to allow episodic delamination.

Because of it's reduced gravitational acceleration relative to the Earth, stretching the solidus and liquidus curves in the depth dimension, Mars may well have a very thick depleted layer in its uppermost mantle. Thermochemical convection calculations of Schott et al. (2001) show a thickness of about 400 km. The Rayleigh number of the martian mantle is difficult to determine, but the interior structure models of Sohl & Spohn (1997) have values of the order of $10^4 - 10^5$. This would marginally allow convection in the lowermost chemical lid only for a non-Newtonian rheology in the large lid slope model. Kiefer (2003) applies higher values on the order of 10⁶–10⁷. Also, a higher Rayleigh number can be inferred for early Mars, and with values of 10^{6} – 10^{7} , a convecting lower chemical lid can easily be obtained. One can construct a speculative scenario in which the demise of convection in the lower chemical lid due to a secular decrease of the mantle Rayleigh number results in a significant reduction of Mars' ability to evacuate heat from the mantle. Continuing this line of thought, this could reduce the heat flow out of the martian core and, therefore, be responsible for the demise of its dynamo.

6.4 Concluding remarks

The results presented in this paper demonstrate that chemical differentiation in planetary mantles does not necessarily change its heat flow characteristics. However, when this heterogeneity results in a stratification, the heat flow is moderately to significantly reduced by a factor of 2–5 compared to non-layered purely thermal convection cases. Therefore, stratified chemical heterogeneities may have important implications for the thermal evolution of terrestrial planets, and the switching off of convection in the chemical lid during the secular cooling of a planet may correspond to profound changes in its rate of heat loss.

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APPENDIX A: NUMERICAL ACCURACY OF THE THERMOCHEMICAL CONVECTION SIMULATIONS

Because of the large number of numerical experiments required for the first part of this work, I have sought a compromise between numerical accuracy (resolution) and computational costs (matrix size and integration time step). The benchmark and resolution tests presented in this appendix demonstrate that resolution was sufficient to warrant a quantitative interpretation of the results.

Fig. 17 shows a time-series of the rms velocity of the code used in this paper for the thermochemical benchmark of Van Keken *et al.* (1997), comparing it to their results. The same resolution has been used as in the numerical experiments of Section 2. The match is quite good up to t = 0.15, where divergence of all tested codes starts to show up.

A number of numerical experiments, including full lid, full remixing, and depleted outer zone cases, were repeated at a higher resolution (resolution of finite element mesh and tracers increased by a factor 1.5 in both directions). Some results are shown in Fig. 18 for three numerical experiments with $Ra = 3 \times 10^5$. Snapshots of temperature and composition and time-series of the Nusselt number and rms velocity are compared (left/black curve: normal resolution; right/grey curve: high resolution). Some divergence is inevitable for long integration times (typical runs have 15 000 integration steps) in a discretized representation of the fields for non-steady states, especially in the chaotic complete remixing case (see thermochemical benchmark comparison in Van Keken *et al.* 1997). However, the results remain qualitatively identical for very long integration times, and the time-series show the same trends long after they have ceased to completely coincide.