DIAPIRISM ON VENUS AND THE EARLY EARTH
AND
THE THERMAL EFFECT OF FLUID FLOWS IN AECL’S TUNNEL SEALING EXPERIMENT

by

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University of Toronto

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Abstract

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Flow instabilities occur at all scales in planetary systems. In this thesis we examine three cases of such instabilities, on three very different length scales.

In the first part, we test the idea that Archean granite-greenstone belts (GGBs) form by crustal diapirism, or Rayleigh-Taylor instabilities. GGBs are characterized by large granitic domes (50-100 km in diameter) embedded in narrow keel-shaped greenstones. They are ubiquitous in Archean (> 2.5 Ga) terrains, but rare thereafter. We performed finite element calculations for a visco-elastic, temperature-dependent, non-Newtonian crust under conditions appropriate for the Archean, which show that dense low-viscosity volcanics overlying a felsic basement will overturn diapirically in as little as 10 Ma, displacing as much as 60% of the volcanics to the lower crust. This surprisingly fast overturn rate suggests that diapiric overturn dominated crustal tectonics in the hot conditions of the Early Earth, becoming less important as the Earth cooled. Moreover, the deposition of large volumes of wet basaltic volcanics to the lower crust may provide the source for the formation of the distinctly Archean granitic rocks which dominate Earth’s oldest continents.

The second part examines the origin of Venusian coronae, circular volcanic features unique to Venus. Coronae are thought to result from small instabilities (diapirs) from the core-mantle boundary, which are typical of stagnant-lid convection. However, most young coronae are located in a region surrounded by long-lived hotspots, typical of a more
active style of mantle convection. Using analogue experiments in corn syrup heated from below, we show that the co-existence of diapirs and long-lived mantle plumes are a direct consequence of the catastrophic overturn of the cold Venusian lithosphere thought to have occurred $\sim 700\, Ma$ ago.

In the last part we analyze the thermal effect of fluid flow through a full-scale experiment testing clay and concrete tunnel seals in a Deep Geological Repository for nuclear waste. Using a commercially available finite element software, we were able to show that the formation of fissures in the heated chamber between the two seals effectively limited heat flow, and could explain the discrepancy between the predicted and measured temperatures.
Acknowledgements

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General Introduction

As is evident from the Abstract, this thesis appears to throw together quite distinct bits of Earth Science Research. The reasons for this are partly beyond my control, and partly personal choice, and require some explanation.

The first 18 months of my PhD were spent continuing a project (the work on Venus) which I began during my M.Sc. under the supervision of Dr. A. Mark Jellinek, who left the university at the end of my first year of graduate school. During my M.Sc. another graduate student (Vid Thayalan) and I installed a new fluid dynamics laboratory whose main project was the analysis of transient convection following the collapse of a stagnant lid during Rayleigh-Bernard convection in corn syrup heated from below and cooled from above. It was a challenging physical set up, and did not run properly until shortly before the end of my M.Sc. As a result, I performed the bulk of the usable experiments (4 of the 5 presented in Part II) in the first term of my PhD before the lab was dismantled, followed by months of data analysis and finally the write up of the publication. These last 4 experiments as well as all the data analysis, scaling, and the text of the publication (except for the numerical work) were done on my own, while consulting with Dr. Jellinek by email and during a week-long work meeting. In the end, the re-write of the publication was significant, and it was not published until 3 years into my PhD (Robin et al., 2007).

Most of my doctoral work was on the Archean crustal diapirism material presented in Part I. This project was developed by Dr. Richard C. Bailey and me before the end of my M.Sc. The finite element code Thermax2D had been written and tested by Dr. Bailey and former graduate student Dr. Jill Pearse. My contributions to the code were the implementation of non-Newtonian rheology and the development of strain modeling. In addition, in consultation with Dr. Bailey, I built the crustal diapirism model, defined the appropriate thermal and rheological parameters, decided which parameters to control, how to analyze the results, and ran all the models. Along the way, I learned a bit of geology, which continues to baffle me with its complexity. Finally, I wrote the text and did all of the analysis for the publication of our results (Robin & Bailey, 2009).

Part III represents a short project taken on as part of the Collaborative Program in Environmental Studies at the University of Toronto’s Center for Environment. In 2007 I decided to see how I could apply my research skills to environmental science research, which led to my application to the Collaborative Program. To fulfill the requirements of the program I took 2 extra courses, and was required to include an environmental
component in my thesis. They felt that the general field of ‘Earth Science’ did not qualify, while I was worried that an extra chapter would not only be too much of a time commitment, but would also be difficult to fit into my geodynamically-inclined thesis. As I was the first person in the Physics Department to join this program, they encouraged me to do something perhaps not traditional in a Physics & Geology PhD. Therefore, after discussing the matter with Dr. Bailey, I approached the Nuclear Waste Management Organization (in Toronto), who suggested looking at the Tunnel Sealing Experiment for something I could apply my thermo-mechanical modeling background to. The resulting choice of project, implementation of modeling, and analysis of results were done on my own, again with consultation with Dr. Bailey.
Part I

Archean Crustal Diapirism
Chapter 1

Introduction

Archean\(^1\) cratons are characterized by granite-greenstone terrains (GGTs), vast areas dominated by massive granitoid bodies interspersed with strips of altered basalt (greenstone belts (GSBs)). GGTs and GSBs are rare in the first half of the Proterozoic, and even rarer in the second half (DeWit & Ashwaal, 1997). Thus they have been the center of a long-standing debate about the evolution of terrestrial tectonics, and in particular, about the operation of vertical vs. horizontal tectonics in the Archean (> 2.5 Ga). Moreover, greenstone belts are host to economically important volumes of gold, base, and rare metal deposits.

Preserved Archean GGTs range in age from \(\sim 2.5 - 3.8\) Ga (Condie, 1989) and are characterized by keel-shaped mafic volcanics 20 to 100 km wide and up to hundreds of kilometers long, interspersed with granitoid domes 50-100 km in diameter (Figures 1.1 and 1.2). In plan view, these synformal greenstones and antiformal granitoid domes resemble salt diapirs, or Rayleigh-Taylor instabilities (MacGregor, 1951; Anhaeusser et al., 1969). Early models and calculations by Mareschal & West (1980) showed that mafic volcanics over a felsic crust imposes the necessary density inversion, and softens the crust by burial of heat producing elements (HPEs) in the felsic unit, leading to the formation of dome-and-keel structures. The time between the deposition of the greenstone supracrustal sequence and the appearance of granitic domes is 20 – 40 \(Ma\) in the Yilgarn and Superior provinces (Rey et al., 2003), suggesting that this is the time needed to ‘conductively incubate’ (Sandiford et al., 2004) the HPE-rich gneissic basement in the

\(^1\)We adopt the definitions of the geological eons as set by the IUGS, as follows: The Neoarchean: 2.5-2.8 Ga; the Mesoarchean: 2.8-3.2 Ga; the Paleoarchean: 3.2-3.6 Ga; the Eoarchean: 3.6-4.0 Ga; and the Hadean: 4.0-4.567 Ga (Van Kranendonk, 2007a).
Figure 1.1: Typical Neoarchean granite-greenstone terrain geology, Kenora District, NW Superior Province, Canada. Map by Blackburn (1981)
Figure 1.2: Paleoarchean granite-greenstone terrain geology, Pilbara craton, NW Australia. From Van Kranendonk et al. (2004).
Chapter 1. Introduction

Neoarchean.

GGT diapirism and predominantly vertical tectonics was a popular model in the 1960’s and 70’s, and has remained popular for the Pilbara (~ 3.5 – 3 Ga) (Collins et al., 1998; Van Kranendonk et al., 2004) and Dharwar (~ 3.3 – 2.5 Ga) (Bouhallier et al., 1995; Chardon et al., 1996, 2002) cratons. However, the age-progressing linear structures and deep-penetrating faults of younger (and larger) Archean terrains such as those of the Superior Province of Canada suggest a modern style of plate tectonics (e.g. Card (1990); Calvert et al. (1995); Thurston et al. (1991)), which has until recently turned the focus away from the diapir hypothesis. Even in the Superior, however, imposing an end-member plate-like model for GGT formation often requires highly unlikely successions of repeated subduction, slab windows, and intermittent plume activity (reviewed in Bédard (2006)), or mechanically implausible shallow subduction (reviewed in Davies (2007)), which have led some to reconsider vertical tectonics.

Indeed, a growing number of researchers feel that the ‘early Earth was a vastly different planet than that of today, primarily due to a higher mantle temperature. Follow-on effects from this include a higher geothermal gradient, which in turn resulted in greater degrees of partial melting of upwelling mantle, a thicker, but softer crust, and a softer, weaker lithosphere’ (Van Kranendonk, 2007a). Archean spreading rates would have been 2-3 greater than today’s (Van Kranendonk, 2007b), giving rise to a thicker oceanic crust and thinner lithosphere. The lithosphere may have been too buoyant to subduct (e.g. Bailey (2006a); Van Kranendonk (2007b)), possibly resulting in ‘trench lock’ (Stern, 2005). In addition, recent modeling suggests that a hot weak lithosphere, even if dense enough to subduct, would easily break off, removing the slab pull force which is a major driver of modern plate tectonics (e.g. van Hunen et al. (2008)). Finally, Archean terrains supply us with little evidence of the common features associated with modern plate tectonics (e.g. ophiolites, blueschists and ultra-high pressure rocks).

Even for those inclined to accept vertical tectonics during the Archean, a ‘starting’ time for the operation of strong plates is not obvious. Stern (2005) finds that the geological record may not be commensurate with modern plates until 1 Ga; others see evidence of plate-like behaviour after 2.1 Ga (Hamilton, 2007). In contrast, Van Kranendonk (2007b) confirms evidence of rifting at the edge of the Pilbara craton beginning at around ~ 3.2 Ga (Van Kranendonk, 2007b), although rifting may be have been local and does not necessarily imply a large-scale rift system as exists today.

In the Superior Province, regional structures are difficult to explain without horizon-
Figure 1.3: Representation of an idealized greenstone belt, based on the Barberton greenstone belt, South Africa. From Anhaeusser et al. (1969).
tal tectonics, and it is generally thought that the various terrains that make it up were accreted in the late Archean. However, significant and rapid vertical displacements are also evident in the Superior’s GGTs (e.g. Lin (2005); Moser et al. (2008)). In other words, Neoarchean GGTs may reflect two length- and timescales operating simultaneously (Lin, 2005; Chardon et al., 2002). Thus, the Superior Province may have captured the transition as the earth cooled and global tectonics evolved from predominantly vertical to predominantly horizontal. This implies an increase in lithospheric strength which is consistent with the secular decrease in radiogenic and secular heating, cooling which may have been aided by the ‘granite bloom’ of 2.5 − 2.7 Ga (e.g. Bleeker (2002)).

Whether this was the case or not, individual dome formation must have been controlled by local thermo-mechanical properties of the crust. Therefore, even without taking sides on the global vertical vs. horizontal debate, it is imperative to understand the thermo-mechanical conditions which allowed for the formation of greenstone-over-granite diapirs. This will be the focus of Chapters 2-4.

A broader question, however, addresses the formation of Archean continents and their associated sub-continental lithospheric mantle (SCLM). The Archean SCLM is unusually thick and buoyant when compared to the SCLM underlying Proterozoic and younger terrains. Archean SCLM has been attributed to imbricated accretion of oceanic or arc-type lithosphere in the context of horizontal tectonics, or the depleted restite of unusually hot mantle plumes in the context of vertical tectonics (reviewed in Lee (2006)). These models are largely based on geochemical arguments, which rely on a priori assumptions about Archean mantle dynamics. Recently, different views on how the mantle may have operated in the Archean have been proposed, partially fueled by similar considerations for the Venusian mantle (e.g. Moresi & Solomatov (1998); Solomatov & Moresi (2000)). For instance, the Archean mantle may have been in an episodic plate-like regime, interspersed between periods of stagnant lid convection (e.g. O’Neill et al. (2007); Davies (2007)), or have been governed by small, low-aspect ratio asthenospheric cells and heavy plume activity (e.g. Ernst (2009)). Such models attempt to address the episodic nature of juvenile crust production (which peaked at 1.1, ∼ 2, 2.7 and 3.5 Ga) (e.g. O’Neill et al. (2007)), and the effect of higher temperatures on mantle circulation. In addition, however, they must also account for geological structures preserved in the crust.

Instead, we may ask the inverse question: could the processes responsible for the formation of such ubiquitous Archean granite-greenstone terrains have been so efficient at crustal reorganization that they can account for the formation of continents and their
SCLM? Such a lithospheric process may have imposed aspects of mantle dynamics from above. Indeed, this would not be unlike the modern Earth’s system of mantle dynamics, which is dominated in planform and heat loss by the thermo-mechanical properties of the lithosphere. Moreover, the preserved mid- to late-Archean greenstone belts we see today reflect a significantly cooler Earth than would have existed in the early Archean and the Hadean; there is no reason to suppose that diapiric structures did not form prior to that. The lack of preserved earlier GGTs may indicate that, on the contrary, diapiric overturn occurred quickly and often in a hotter, more ductile crust. Hence, we can speculate that vertical tectonics, made possible by crustal diapirism at the surface, may have been the first Terrestrial mode of tectonics following the primal magma ocean. This will be discussed in Chapters 5 and 6.

1.1 Geological Setting

Major granite greenstone terrains are found in the Superior and Slave Provinces (Canada), the Zimbabwe and Kaapvaal Provinces (Africa), the Dharwar craton (India), the Yilgarn and Pilbara Provinces (Australia), in Finland and Russia, and in Wyoming (USA) (Condie, 1989; Windley, 1999). Early work emphasized their similarities, while in the late 70’s and 80’s much was made of their differences (Windley, 1999). Our models are by nature simple in design, and thus we address the unifying features of GGTs. In detail, of course, crustal diapirism may behave quite differently due to local structural, mechanical, petrological and thermal heterogeneities. In addition, other tectonic mechanisms, whether simultaneous with or post-dating diapirism, also contribute to the final and preserved state of GGTs. Thus while we address general features common to most GGTs, we do not deny the importance of the differences between them.

1.1.1 Greenstone Belts

Greenstone belts consist of low metamorphic grade mafic to ultramafic metavolcanics interbedded with lesser volumes of metasediment, bordered and intruded by granites. The volcanics become progressively less mafic upwards through each stratigraphic sequence, often including felsic metavolcanics in the upper strata. The stratigraphic sequence may be repeated several times in the GSB (Ayres & Thurston, 1985; Thurston et al., 1991). Total stratigraphic thickness is typically $\sim 10 - 20$ km (DeWit & Ashwaal,
1997), although thicknesses up to 40 km have been observed (Ayres & Thurston, 1985). Geophysical observations (gravity, magnetic and seismic) indicate that preserved keels may extend down to 12 km depth or more, but are more typically 5 – 6 km deep (Peschler et al., 2004; Nitescu et al., 2006), and this range of depths has remained more or less the same throughout the Archean (Peschler et al., 2004).

Preserved mafic units in GSBs contain up to 20% komatiite, a dense, ultramafic rock characterized by its unusual spinifex texture and its low melt viscosity (Arndt, 1983). Komatiite is thought to have formed by high degrees of melting of hot mantle (\(\sim 1600^\circ C\)), implying a source depth on the order of 150 km, although the origin of komatiitic melts remains controversial (e.g. Grove & Parman (2004)). Its production has fallen off drastically since the Archean (DeWit & Ashwaal, 1997). Indeed, the early Archean crust may have been significantly more komatiitic than what is observed today (Arndt, 1983), and the decrease in apparent production of komatiite before \(\sim 3\) Ga (when the mantle was hotter) may be a result of preservation biases. Thus komatiite is thought to be an important indicator of Archean tectonics and mantle dynamics.

The majority of GSBs are inferred to have formed subaqueously (Nisbet, 1982; Arndt, 1983; Thurston et al., 1991). For instance, they often preserve pillow basalts, and are characterized by chloritized basalt. Hydrous alteration also caused komatiites to be typically between 10% and 100% serpentinized (Arndt, 1983).

In the words of P.C. Thurston, ‘Archean greenstone belts have almost universally enjoyed deformation’ (Thurston, 2002). GSBs are highly strained synforms with near vertical dips, with strata typically younging away from the granite-greenstone contact, and with symmetric stratigraphy across the center of the keel (e.g. Bouhallier et al. (1995); Van Kranendonk et al. (2004); Parmenter et al. (2006)). They may also contain late, discordant felsic plutons (Figure 1.3) (Condie, 1981). Where basement contacts are known, it appears that greenstones generally erupted onto older gneissic basement, although the basement itself may also include greenstones (Condie, 1981), implying a previous generation of greenstone volcanism.

### 1.1.2 Granitoid Domes

As their name implies, granitoid bodies surrounding GSBs are anticlinal domes circular to elliptical in shape. Internally, they are highly complex structures often resulting from the solid-state rise of gneissic basement followed by later intrusions (e.g. Schwerdtner et al.
In other cases, granitic intrusion was coeval with the doming (e.g. Sandiford et al. (2004)). Indeed, dome amplification by melt intrusion lasted up to $\sim 700 \text{Ma}$ in the Pilbara (Van Kranendonk et al., 2004). In older terrains, granite batholiths extend down to $\sim 10 \text{km}$, while for younger terrains the batholiths are more tabular, with poorly defined roots at $\sim 5 - 6 \text{km}$ (Peschler et al., 2004; Nitescu et al., 2006), suggesting an evolution in the intrusive mechanisms (Peschler et al., 2004). In addition, batholiths may include crescent-shaped slices of greenstone embedded in their domical structure (e.g. Schwerdtner (1989)), which suggests they may have formed as repeated tabular intrusions before or during doming (Cruden & Robin, 1998). Their structural complexity has made it difficult to determine the primary tectonic mechanism responsible for their formation (see Chapter 4).

Most Archean batholiths are made of tonalite-trondhjemite-granodiorite (TTG) which make up the bulk of Archean continental cratons, but whose origins are still debated. TTGs are granitoid rocks which are distinguished from later granites by their unusually depleted heavy rare earth elements (HREE) signature and low potassium content. Since garnet strongly fractionates HREE, TTG probably result from partial melting of wet metabasalts in the garnet stability field (e.g. Moyen & Stevens (2006)), leaving a dense restite rich in garnet. There are two likely pressure-temperature conditions for TTG formation: at 8-15 kbar and 700-1000 C (for instance, at the base of a thickened oceanic crust), or at 15-25 kbar and 700-900 C (for instance, from the top of a subducting slab) (Moyen & Stevens, 2006). Some later Archean granite domes are more potassic, and may have formed by remelting of older TTG crust (e.g. Bédard (2006); Van Kranendonk et al. (2004)). Thus the origin of TTG is also an important part of the early Earth tectonics debate.

1.1.3 The Hadean

The oldest dated minerals discovered to date are the Jackson Hill detrital zircons from Western Australia ($\sim 4.4 \text{Ga}$) (Wilde et al., 2001), while the oldest rocks are the Acasta gneisses from the Slave Province of Canada ($\sim 4.03 \text{Ga}$) (Condie, 2007; Kamber, 2007). The recently measured $^{142}\text{Nd}/^{144}\text{Nd}$ ratio of the Nuvvuagittuq greenstone belt (Quebec) suggests that the rocks themselves or their parent source rock were formed at $\sim 4.28 \text{Ga}$ (O’Neil et al., 2008). In addition, radiogenic isotope evidence for volcanic resurfacing as early as 4.4 Ga and calculations of resulting thermal profiles suggest that mafic crust
Chapter 1. Introduction

existed at 4.35 Ga (Kamber et al., 2005). This early protocrust would have differentiated if it reached \( \sim 40 \) km, leading to compositional stratification and the formation of zircon-bearing felsic rocks (Kamber et al., 2005; Kamber, 2007).

Thus, density stratification and volcanic resurfacing is likely to have occurred quite early in the Hadean. As a result, crustal density inversions similar to those of our starting models could have been present much earlier than the earliest preserved GGTs (\( \sim 3.8 \) Ga). We will show that diapirism may have been the inevitable result.
Chapter 2

Numerical Experiments

We performed fully coupled thermal and viscoelastic mechanical modeling of an inverted density profile, using a geometry and density stratification similar to that of Mareschal & West (1980).

Due to computational limitations, the models of Mareschal & West (1980) were limited to high thermal inputs and a restricted range in viscosities. In addition, their rheological laws are neither stress-dependent nor visco-elastic. Nevertheless, they were able to reproduce the general morphology and strain distribution of a GGT diapir (Figure 2.1), as well as the skewed thermal profile as cold temperatures are advected downwards in the keel and warm temperatures upwards in the dome. Their numerical results are still referenced in models of GGT formation by diapirism (Figure 2.2).

Our preliminary results showed significant differences from those of Mareschal and West, in particular regarding the rate and shape of diapir formation. We attribute these differences to more advanced meshing techniques and higher-order interpolation schemes of our finite element program (Thermax2d). For our final models, we expanded their model to include non-Newtonian rheologies and a broad range in viscosities, as well as elasticity.

2.1 Physical Model

Each calculation begins with a thermally equilibrated felsic layer of thickness 15 km over a mafic layer of modeled thickness 10 km (Figure 2.3). At time $t = 0$, a 10-km layer of mafic or ultramafic volcanics is considered to be emplaced on top, in a negligible time. This is a simplification of the fast deposition of volcanics as many thin subacqueously-
cooled flows, and the starting temperature of this supracrustal layer is thus taken as 0°C. The suddenness of this supracrustal addition is not important to the subsequent physics, but makes the definition of a starting time simpler. Indeed, the inclusion of realistic rates of supracrustal volcanism will lengthened the time to overturn, but not as much as might be concluded by simply adding the volcanic accumulation time to the instability growth time, since both heating and overturn begin before the 10 km of volcanics are fully deposited.

The model’s thermal evolution is controlled by the competition between two processes,

Figure 2.1: Details of the model set up and mesh for the crustal diapir calculations of Mareschal & West (1980)
each with its own time scale: conductive re-equilibration, and advective (diapiric) disequilibrium. If diapirism were absent, the thermal state would evolve from an initial geotherm to a final geotherm (Figure 2.4). In reality, the thermal profile through the downwelling part of the diapir is significantly cooler than that in the upwelling part (Figure 2.4 inset).

Our model is 50-km-wide, 35-km-deep, and contains a basal mafic layer (of density $\rho = 2900\, \text{kg/m}^3$), a middle granitic layer ($\rho = 2700\, \text{kg/m}^3$), and an upper mafic layer ($\rho = 2900\, \text{kg/m}^3$). The top of the model is stress free and held at $0^\circ \text{C}$. The sides are periodic, and the bottom has a zero velocity boundary. In detail, we calculated only half the model for computational efficiency, but the use of symmetric boundary conditions mean that our models represent an infinite series of diapiric structures (Figure 2.3).

![Diagram](image)

Figure 2.2: Results taken from Figure 4 of Mareschal & West (1980), as presented in Figure 6 of Collins et al. (1998). The final configuration shown in (c) and (d) represents the overturn 17.7 Ma after the initial volcanic deposition. In (d) the lines represent accumulated strain.
A sinusoidal interface is imposed on the interface between the upper and middle layers, given by

\[ A = A_0 \exp\left(\frac{2\pi x}{\lambda}\right) \]  \hspace{1cm} (2.1)

where \( A_0 \) is amplitude (here, 400 m), \( x \) is distance along the horizontal axis, and \( \lambda \) is the wavelength (here, 50 km).

The width of our models was chosen based on the typical width of GGT domes, and on the stability analyses of Mareschal & West (1980) and de Bremond d’Ars et al. (1999); a suite of models testing different wavelengths confirms that 50 km is an appropriate choice (Chapter 3.2.5). Their calculations were based on the formulations of Artyushkov (1971) for a two-layered system and Ramberg (1981) for a multi-layered system, respectively. Indeed, analytic and numerical calculations of the growth of Raleigh-Taylor instabilities have been published for a variety of boundary conditions, density structures and for Newtonian and non-Newtonian rheologies (e.g. Danes (1964); Selig (1965); Biot & Odé (1965); Ramberg (1967, 1968); Artyushkov (1971); Conrad & Molnar (1997); Houseman & Molnar (1997)). Such analyses solve for the dominant wavelength \( \lambda \) and growth rate of sinusoidal perturbations in the case where the amplitude/wavelength ratio (\( \eta/\lambda \)) is small (less than 5-10% (Ramberg, 1981)). A sinusoidal perturbation between layers of densities \( \rho_1 \) (upper layer) and \( \rho_2 \) (lower layer) (where \( \rho_1 > \rho_2 \)) will grow exponentially with time according to

\[ A = A_0 \exp(st) \]  \hspace{1cm} (2.2)

where \( s \) is the rate of growth which depends on the density contrast \( \Delta \rho \), the ratio of wavelength to the depth of the top layer \( \lambda/h_1 \), the ratio of the two layer depths \( h_2/h_1 \), the viscosity ratio of the two layers \( \eta_1/\eta_2 \), the boundary conditions, and, in the case of non-Newtonian viscosities, the stress exponent. The growth rate is determined by a competition between the gravitational force driving the flow, and the viscous resistance to the growth of the instability in both layers. Thus, for large \( \lambda/h_1 \), growth rate will be limited by the resistance to large lateral motions in the top layer, while for short \( \lambda/h_1 \), growth rate will be limited by the ability of the lower layer to accommodate large volumes of flow from the upper layer (i.e. \( h_2/h_1 \)). In general, the use of temperature- or stress-dependent viscosities slows growth rates because the amount of material involved in the instability is limited to a thin layer above the interface (Houseman & Molnar, 1997).
Internal heating \((H)\) by heat-producing elements (HPEs) is included as an evenly distributed source in the granitic layer only, since the concentration of U, Th and K are roughly 100 times greater in granites than they are in basaltic rocks. In addition, a constant heat flux is imposed at the base of the model, simulating heat flux from the mantle \((q_m)\).

### 2.2 Thermal inputs

Archean thermal parameters are generally poorly constrained. Estimates of crustal heat productivity by the decay of heat producing elements (HPE) are based on measurements of current concentrations of K, Th and U in cratonic crust, and then extrapolation back in time using the relationship

\[
H = H_0 \exp \left( \frac{t \ln(2)}{\tau_{1/2}} \right)
\]  

(2.3)

where \(H\) is the current concentration of the heat-producing isotope, \(H_0\) is the concentration at time \(t\), and \(\tau_{1/2}\) is the half-life of the isotope (Turcotte & Schubert, 2002). Summed over the isotopes \(^{238}U\), \(^{235}U\), U and K, this gives heat production rates of \(\sim 2\) times today’s rate at 2.55 Ga and \(\sim 3\) times today’s rate at 3.55 Ga (Bailey, 2006a; Mareschal & Jaupart, 2006). Thus, if the current HPE content of Archean rocks is known, we should know their heat productivity during the Archean.

However, measuring \(H\) is fraught with difficulties and assumptions. For instance, since HPEs are largely fractionated to melts, felsic rocks contain most of the HPEs in the crust, and are typically in the upper crust. In detail, the distribution of HPEs in the crust depends on local geology, and must be extensively sampled. In addition, the depth distribution of HPEs is rarely uniform, or even exponentially decreasing (Jaupart & Mareschal, 1999; Mareschal & Jaupart, 2006).

Indeed, measured values can vary greatly within and between cratons. The average present-day surface heat production in the Yilgarn Province (Australia) is \(3.3 \, \mu W/m^3\), although locally can reach values of \(> 8 \, \mu W/m^3\), while in the Superior Province (Canada), average present-day surface heat production is \(\sim 1 \, \mu W/m^3\) (Mareschal & Jaupart, 2006). Therefore, average heat production of the late Archean could have ranged from \(\sim 2.5 \, \mu W/m^3\) in the Superior to \(\sim 7 \, \mu W/m^3\) in the Yilgarn, and locally could have reached up to \(\sim 20 \, \mu W/m^3\)! In the Hadean and early Archean, heat production would have been
Figure 2.3: Model set-up: Here, $\sigma_t$ is stress tangential to the boundary, $\sigma_n$ is stress normal to the boundary, $\rho$ is density, $v_n$ is velocity normal to the boundary, $H$ is the concentration of HPEs, $q_m$ is mantle heat flux, $T$ is temperature, and $t$ is time. For all models, the bulk modulus $\mu$ and shear modulus $K_b$ are 30 GPa. The rheological properties used are given in Table 2.1.
even higher. For the purpose of our general models, we test a values of $H$ between 3 and 10 $\mu W/m^3$. However, imposing an average global thermal regime probably does not represent any specific Archean craton (Mareschal & Jaupart, 2006).

Estimates of current mantle heat flux are made by taking the total crust heat flux ($q_c$) and removing the estimated crustal heat production, using the simple (and rarely observed) heat flow to heat production relation

$$q_c = q_m + HD$$

where $D$ is the depth of the HPE-enriched layer. For Archean cratons, present-day values of $q_m$ are 10-17 $mW/m^2$.

Unfortunately, there is no direct way to know what the mantle contribution would have been in the Archean, which has to be estimated based on other considerations. In general, there is a sense that heat production, and therefore $q_m$, would have been higher during the Archean (e.g. Bodorkos & Sandiford (2006)). Moreover the cold sub-continental lithosphere may not have been as thick during the formation of the crust, although it may have grown during the process. For a hotter mantle and thinner lithosphere, the application of Fourier’s law

$$q_m = -k \frac{dT}{dz}$$

suggests that $q_m$ could have been considerably higher in the Archean (where $k$ is the thermal conductivity, $T$ is temperature and $z$ is depth). Based on these considerations, some authors use values of $q_m = 35$ $mW/m^2$ (Bodorkos & Sandiford, 2006).

On the other hand, since cratons remained stable during and since the Archean, mantle temperatures and heat flow beneath the Moho may not have been much higher than they are today. A more quantitative approach is to estimate Archean mantle temperatures based on the T-P conditions constrained by preserved mantle-derived rocks. However, the origin of these rocks (whether high-T, low-P or vice-versa, or wet vs. dry) is still debated, and estimates of mantle temperatures range from 7-40% hotter than today’s. Based on these arguments, Mareschal & Jaupart (2006) estimate $q_m$ during the Archean at 13 - 20 $mW/m^2$, and Bailey (2006a) uses a value 10% greater than today’s.

We model values of $q_m$ from 15 to 40 $mW/m^2$. Fortunately, as long as this number is within a reasonable range, uncertainty in $q_m$ is not a great concern, since our models show that the most important thermal parameter in our models is $H$, the concentration of HPEs.
We also considered a number of other constraints. For instance, total crustal heat flux \(q_c\) over sizeable areas today are as high as 110 mW/m\(^2\) Bailey (2006a), and locally can be higher. Also, Archean granitoid domes were often intruded by melt, or formed as successive melts of the basement TTG layer (e.g. Van Kranendonk et al. (2004); Béard (2006)), implying that the base of the domes and/or the crust should be near the solidus (\(\sim 1000^\circ C\) for basalt, and \(\sim 700^\circ C\) for granite).

Based on these constraints, we model three sets of thermal parameters shown in Figure 2.4 (for details on how these are calculated, see Appendix A). In this figure we show two sets of geotherms. The initial geotherm is shown with the top 10 km at 0° C. If no overturn occurs, it evolves to the final geotherm. Using Equation 2.4, our values yield Archean surface heat flow values of 80 – 190 mW/m\(^2\). For our intermediate thermal profile, we achieve final equilibrium temperatures of 800° C at 20 km depth, implying some degree of melting at the base of the dome. Our ‘hot’ thermal profile is clearly unstable, as the bottom of crust is past the liquidus of basalt (\(\sim 1200^\circ C\)), primarily due to the high concentration of HPE’s.

However, it is important to note that the final equilibrium temperatures are rarely reached. As the model evolves from the initial to the final geotherm, the rheology is softened up and the system overturns. Thus, the actual final geotherm is hotter in the rising dome than it is in the sinking keel. This serves to protect the mechanical integrity of the greenstone keel, while allowing melting at the base of the dome.

Interestingly, even higher values than those of our ‘hot’ thermal profile have been observed (see above). Preservation of these features to the present day suggest that removal of these middle HPE-rich layers to the upper crust (i.e. crustal reorganization) must have occurred very quickly.

### 2.3 Rheological parameters

We use 3 distinct non-Newtonian rheologies in each of the three layers (see Table 2.1) based on the standard definition of viscosity (Equation 2.11). Our choice of rheologies is based on the work of de Bremond d’Ars et al. (1999). Their numerical stabilities analysis suggested that in order to amplify wavelengths on the order of 50-100 km (a typical dome size in GGTs), the ratio of viscosities between the supracrustal volcanics and granitoid layer must be \(10^{-3}\) to \(10^{-4}\). To achieve this viscosity contrast, they call on the hydrous alteration of the volcanic sequence, in particular of the ultramafic or komatiitic flows.
Figure 2.4: Thermal regimes. We test a set of 3 geotherms with the following parameters: "hot": $H = 10 \mu W/m^3$ and $q_m = 40 mW/m^2$; "intermediate": $H = 7 \mu W/m^3$ and $q_m = 25 mW/m^2$; and "cold": $H = 5 \mu W/m^3$ and $q_m = 15 mW/m^2$. For all calculations, thermal diffusivity ($\kappa$) is $1 \times 10^{-6} m^2/s$. Thermal conductivity ($k$) is $2.4 W/m/K$ for the "hot" case and $2.7 W/m/K$ for all other cases.
Komatiite is rich in olivine and is readily serpentinized in the presence of water. This increases its ductility and decreases its density. de Bremond d’Ars et al. (1999) argue that the rate of serpentinization is comparable to the rate of deposition of oceanic basalts. Therefore, even if GSBs contain only up to 20% komatiite (see 1.1.1), the viscosity of the supracrustal sequence will be controlled by serpentinite, its weakest constituent.

Moreover, komatiites tend to form the first stratigraphic layers, placing them at the most active part of the upper layer where it is in contact with the middle layer. Thus, because it is the weakest phase and is found at the key location above the mafic-felsic interface, moderate amounts of altered komatiite will determine the bulk rheological response of the volcanic sequence without greatly decreasing bulk density.

In addition, basaltic volcanism is similarly weakened by the hydrothermal alteration, which, along with low-grade metamorphism, gives greenstones their characteristic colour (W.M. Schwerdtner and P.-Y. Robin, personal communication). Unfortunately, no rheological law is available for greenstone.

Consequently, we start with the rheological parameters for serpentinite in the upper layer (Raleigh & Paterson, 1965), and a density contrast of 200 kg/m³ (7%) between the upper two layers. This density contrast is chosen based on the work of Mareschal & West (1980) and confirmed by the measured averages of Peschler et al. (2004) and the analysis of de Bremond d’Ars et al. (1999). We explore the effect of decreasing alteration of the volcanic sequence by varying the rheological parameters of the serpentinitic upper layer to approach those of unaltered mafic volcanics. For the altered volcanics, we use the parameters given by Raleigh and Patterson (1965) for the Tumut Pond Serpentinite. We model unaltered mafic volcanics using the parameters for diabase given by Caristan (1982), which we also use in the lower layer for all models. For the granitic layer, we use a quartz-diorite rheology (Hansen & Carter, 1982) (see Table 2.1 and Figures 2.3).

<table>
<thead>
<tr>
<th>Source</th>
<th>$A$</th>
<th>$Q$</th>
<th>$n$</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>diabase</td>
<td>$6 \times 10^{-2} \text{s}^{-1} \text{MPa}^{-n}$</td>
<td>$276 \text{kJ/mol}$</td>
<td>3.05</td>
<td>Caristan (1982)</td>
</tr>
<tr>
<td>quartz-diorite</td>
<td>$3 \times 10^{-2} \text{s}^{-1} \text{MPa}^{-n}$</td>
<td>$212 \text{kJ/mol}$</td>
<td>2.45</td>
<td>Hansen &amp; Carter (1982)</td>
</tr>
<tr>
<td>serpentinite</td>
<td>$6.3 \times 10^{-7} \text{s}^{-1} \text{MPa}^{-n}$</td>
<td>$66 \text{kJ/mol}$</td>
<td>2.8</td>
<td>Raleigh &amp; Paterson (1965)</td>
</tr>
</tbody>
</table>

Table 2.1: Rheological parameters.
These rheologies were used based on the modeling of de Bremond d’Ars et al. (1999). Other rheological laws are available, in particular for wet and dry diabase (Mackwell et al., 1998); however, the rheology of diabase in its unaltered state was only used in the lowest layer, which played an insignificant role in the overturn evolution. In the upper layer, the law for unaltered wet diabase was already sufficiently viscous to inhibit diapiric overturn on a reasonable time scale. Hence, the use of a stiffer (dry) rheology would not have changed our results.

2.4 Finite Element Code

Our models were performed using Thermax2d, a 2-dimensional finite element program based on the commercially available package FEMLAB (Bailey, 2006b; Pearse, 2005). It has a moving mesh, and a large time-stepping algorithm that allows it to solve viscoelastic constitutive relations on a single processor.

The momentum equation for non-inertial flows is given by

$$\frac{\partial \sigma}{\partial x} + F = 0$$ (2.6)

where $\sigma$ is the stress tensor, $F$ is the body force, and $x$ are the spatial coordinates. For an isotropic elastic solid, stress is given by

$$\sigma = \lambda Tr(\varepsilon)I + 2\mu \varepsilon$$ (2.7)

where $\varepsilon$ is the strain tensor, $I$ is the identity matrix, $\mu = G$ is the shear modulus and $\lambda$ is Lamé’s second parameter (in terms of the bulk modulus $G$, $\lambda = K - \frac{2}{3}G$). For a Newtonian viscous solid,

$$\sigma^{(D)} = 2\eta \dot{\varepsilon}^{(D)}$$ (2.8)

where $\eta$ is the viscosity, and $\dot{\varepsilon}$ is the strain rate, and $D$ indicates the deviatoric part of the tensor. For an isotropic linear viscoelastic solid, the material is modeled as a dashpot and a spring connected in series, and its constitutive relation is
\[
\dot{\sigma}^{(D)} + \frac{\sigma^{(D)}}{\tau} = 2\mu \dot{\varepsilon}^{(D)}
\]  

(2.9)

where \( \tau = \eta/\mu \) is the Maxwell viscoelastic relaxation time. Thus, when \( t < \tau \), the material behaves elastically, whereas when \( t > \tau \), the material behaves viscously.

However, a problem arises when solving this equation, as the timescale for elastic deformation and for viscous deformation span several orders of magnitude for rheologies encountered in the crust. This imposes inconveniently small times steps on the calculation in order to guarantee stability and/or accuracy. Thermax2d avoids this by taking time steps which are small based on the timescale of deformation (the ‘tectonic’ time scale), defined as the timescale over which the strain rate is effectively constant, as opposed to the Maxwell relaxation time. More details of the time-stepping algorithm and its application in Thermax2d can be found in Bailey (2006b) and Pearse (2005).

In practice, a convenient set of output time steps are input by the user, along with acceptable degrees of deformation for each time step (entered as fractional changes in element dimensions). Thermax2d then attempts to solve the equations for the defined time step, but reduces the time step if it results in greater deformation than allowed. In some cases, a single user-defined output time will take 100 or more attempts by Thermax2d as it tries to accommodate the deformation constraints; this ‘guessing’ for an appropriate time-step is the most expensive part of the calculation, in particular during the active overturn phase. To avoid this, we modified Thermax2d to allow for a pre-defined number of time-step per output interval. However, this did not significantly reduce calculation time, as the model spanned a large range of different strain rates (with most of the deformation occurring in a relatively short time), so that the time saved on ‘guessing’ the smaller time steps was lost when small time steps were not needed.

In our models, viscosity \( \eta \) depends on temperature, given by the thermal diffusion equation:

\[
C_v \frac{\partial T}{\partial t} = k \nabla^2 T + H
\]

(2.10)

where \( C_v \) is the volumetric heat capacity, \( T \) is temperature, \( t \) is time, \( k \) is thermal conductivity and \( H \) is internal heat productivity per m\(^3\). Advection of heat is not calculated...
explicitly, as heat is advected by the moving mesh.

### 2.4.1 Non-Newtonian rheology

After testing the Mareschal & West (1980) model, we configured Thermax2d for stress-dependent (i.e. non-Newtonian) viscosities, describing a highly stress-dependent mechanism of creep dominated by the movement of lattice dislocations. Stress- and temperature-dependent rheologies are approximated as

$$
\dot{\varepsilon} = A e^{-Q/RT} \sigma^n
$$

-giving the following definition of viscosity:

$$
\eta = \frac{\sigma}{2\dot{\varepsilon}} = \frac{1}{A e^{-Q/RT} \sigma^{n-1}}
$$

When $\sigma$ is $\sim 0$, however, $\eta$ is undefined and the computation fails. In addition, extremes in viscosity are both computationally undesirable and physically unrealistic. Therefore, we adopt the following formulation for viscosity:

$$
\eta = \eta_{\text{min}} + \frac{1}{\eta_{\text{max}} + \eta_{\text{Newt}}(T) + \eta_{\text{Non-Newt}}(\sigma,T)}
$$

where $\eta_{\text{Non-Newt}}(\sigma,T)$ is defined by Equation 2.12. $\eta_{\text{Newt}}(T)$ (Newtonian viscosity) describes viscous flow dominated by diffusion creep, which is highly sensitive to temperature but not significantly sensitive to stress. We include Newtonian viscosity because at low stresses (10-100 MPa (Ranalli (1995))), flow is dominated by temperature-dependent processes (diffusion creep) rather than stress-dependent ones (dislocation creep). Thus we define $\eta_{\text{Newt}}(T)$ by setting the stress exponent $n$ in $\eta_{\text{Non-Newt}}(\sigma,T)$ to 1, and varying the scaling term $A$ for each viscosity law such that the stress-dependent rheology and the temperature-dependent rheology are equal at 30 MPa. In effect, then, at low stresses, $\eta_{\text{Non-Newt}}(\sigma,T)$ becomes small and the flow is dominated by $\eta_{\text{Newt}}(T)$.

$\eta_{\text{max}}$ and $\eta_{\text{min}}$ represent physical upper and lower limits on our effective viscosity. In practice, they are reached only at extremes of temperature and stress, when $\eta(\sigma,T)$ would otherwise be unrealistically high or low for solid-state crustal processes. $\eta_{\text{min}} = 10^{16} \text{ Pas}$
is the estimated viscosity of the mobile lower crust under the Tibetan plateau (Royden et al., 2008). $\eta_{max} = 10^{28} \text{Pas}$ represents a brittle upper crust where viscous deformation is so slow that it is effectively zero.
Chapter 3

Results: Morphology and Overturn Time

All of our models replicate the bulk morphology of GGTs - that is, anticlinal felsic domes and synclinal mafic keels (e.g. Figures 3.1 to 3.3). In this chapter we present our initial results before moving on to stress-dependent models, for which we systematically varied a number of controlling parameters.

3.1 Initial results

The aim of our first models was to reproduce the results of Mareschal & West (1980) using a coarse mesh, no elasticity, and Newtonian viscosities. At this stage we adopted their thermal parameters (which become our ‘hot’ thermal profile), and the viscosity law

\[ \eta = 0.50 \times 10^{20} \exp(2000/T) \, Pa \cdot s \]  

This defines a rheology with an activation energy \( Q \) much lower than expected for granite or even altered greenstone, but was imposed on Mareschal & West (1980) by computational limitations. We forced our initial models to be purely viscous by imposing bulk and shear moduli of \( 10^{10} \, Pas \), giving Maxwell relaxation times of \( \sim 100 \, s \). We attempted to emulate the coarse mesh as closely as possible; however, beyond a certain mesh deformation, Thermax2d refines the mesh automatically.
Our models show finer details, with narrower keels and fine structures in the overturned keel, than the equivalent Mareschal & West (1980) ones (Figures 3.1 and 3.2). In addition, we were unable to reproduce the overturn time using the same rheological parameters - for the same parameters, our models took $\sim 40\%$ longer to overturn (Figure 3.1; compare to Figure 2.2).

We tested a number of models with and without elasticity, and for different scaling parameters $A$ and activation energies $Q$. In Figure 3.2 we show the result for a model with the viscosity law

$$\eta = 0.50 \times 10^{22} \exp(4000/T) \text{ Pa} \cdot \text{s}$$

which is still a low activation energy for most rocks. Despite this low $Q$ and the high thermal inputs, this is quite a slow overturn with respect to our final results presented below.

We attribute the differences between our models to the refined mesh imposed by Thermax2d and to the higher order interpolation scheme. Our initial models also show a level of detail in the head of the descending keel 'plume' which is more than expected, probably as a result of the fact that the same viscosity is used throughout. The lack of viscosity contrast between the two layers as well as the lack of elasticity enabled finer features than our more realistic models achieved. Nevertheless, the general similarity of the our results to theirs was an encouraging start.

### 3.2 Final models

After implementing non-Newtonian viscosity in Thermax2d (Chapter 2.4.1), defining the thermal and rheological parameters of interest (Chapter 2.2), and testing a generic model for diapirism, we examined the influence of rheology and thermal regime on overturn time and morphology. Models were calculated on a PC, and took anywhere from 3 hours to 3 weeks to run, depending on the rheology and choice of output time intervals. In general, elastic and Newtonian models were faster to calculate than purely viscous and non-Newtonian ones, due to the localization of deformation in the latter two. The results
Figure 3.1: Our calculation of a crustal diapir using the same temperature-dependent Newtonian viscosity as that used for Figures 3 to 5 in Mareschal & West (1980).
Figure 3.2: The same model as that shown in Figure 3.1, using an activation energy $Q$ twice as high as that used for Figures 3 to 5 of Mareschal & West (1980).
Table 3.1: Parameters available in Thermax2d. Each domain is assigned its own set of parameters individually. Moduli of $10^{10}$ Pas were used for purely viscous models.

shown here represent 400-500 hours of CPU time, and only about one-fifth of the models calculated over the course of this project.

To quantify the differences between models we define two parameters: $\tau_{20}$, the time in millions of years for a keel to reach 20 km depth (the sum of a typical greenstone depth (Peschler et al., 2004) and an assumed 10 km of erosion); and K:D, the ratio between keel and dome width at 10 km depth (the presumptive depth of later erosion), measured at time $\tau_{20}$. For most models, the keel eventually pinches off; K:D is therefore indicative of the volume of supracrustal material transported to the lower crust.

Table 3.1 lists all of the parameters available in Thermax2d, and Tables 3.2 to 3.6 summarize the results of the important model runs. Each table includes the results for variations of a different control variables.

### 3.2.1 Overturn Evolution

Figure 3.3 shows the evolution of a typical crustal diapir. This model is visco-elastic, using the stress-dependent parameters for serpentinite in the upper layer, and our intermediate thermal parameters ($H = 7 \mu W/m^3$ uniformly distributed in the granitic layer and $q_m = 25 W/m^2$). In B we show the keel at 20 km depth, which is our reference depth for the definition of $\tau_{20}$ as well as the stage at which we measure $K : D$. The line at 8 km depth (shown in A and B) has no physical significance and is a marker horizon embedded in the material. We include it to outline the advection of material from the lowest portion
Figure 3.3: Typical overturn evolution. Colour represents viscosity on a log scale and velocity is indicated by black arrows.
### Table 3.2: Control variable: $H$ (internal heating). Cold start: initial geotherm corresponds to the thermal regime $H = 5$, $q_m = 15$, $k = 2.4$ for all runs.

<table>
<thead>
<tr>
<th>Run</th>
<th>$H$ (µW/m²)</th>
<th>$q_m$ (mW/m²)</th>
<th>$k$ (W/m/K)</th>
<th>$Q$ (kJ/mol)</th>
<th>$A$ (MPa⁻¹)</th>
<th>$q_c$ (mW/m²)</th>
<th>$\tau_{20}$ (Ma)</th>
<th>K:D</th>
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<td>H1c</td>
<td>3</td>
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<td>2.7</td>
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<td>106</td>
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<tr>
<td>H2c</td>
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<td>25</td>
<td>2.7</td>
<td>66</td>
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<td>H4c</td>
<td>5</td>
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<td>2.7</td>
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<td>H5c</td>
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<td>0.51</td>
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<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>160</td>
<td>9.8</td>
<td>0.65</td>
</tr>
<tr>
<td>H9c</td>
<td>10</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>175</td>
<td>8.4</td>
<td>0.59</td>
</tr>
</tbody>
</table>

### Table 3.3: Control variable: $H$ (internal heating). Equilibrium temperature start, using different $H$ and $q_m$ for each starting run.

<table>
<thead>
<tr>
<th>Run</th>
<th>$H$ (µW/m²)</th>
<th>$q_m$ (mW/m²)</th>
<th>$k$ (W/m/K)</th>
<th>$Q$ (kJ/mol)</th>
<th>$A$ (MPa⁻¹)</th>
<th>$q_c$ (mW/m²)</th>
<th>$\tau_{20}$ (Ma)</th>
<th>K:D</th>
</tr>
</thead>
<tbody>
<tr>
<td>H1</td>
<td>3</td>
<td>35</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>80</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>H2</td>
<td>3</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>70</td>
<td>1067</td>
<td>0.51</td>
</tr>
<tr>
<td>H3</td>
<td>4</td>
<td>26</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>86</td>
<td>61.3</td>
<td>0.54</td>
</tr>
<tr>
<td>H4</td>
<td>5</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>100</td>
<td>27.6</td>
<td>0.56</td>
</tr>
<tr>
<td>H5</td>
<td>6</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>115</td>
<td>17.4</td>
<td>0.57</td>
</tr>
<tr>
<td>H6</td>
<td>7</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>130</td>
<td>11.4</td>
<td>0.60</td>
</tr>
<tr>
<td>H7</td>
<td>8</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>145</td>
<td>8.55</td>
<td>0.57</td>
</tr>
<tr>
<td>H8</td>
<td>9</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>160</td>
<td>6.4</td>
<td>0.59</td>
</tr>
<tr>
<td>H9</td>
<td>10</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>175</td>
<td>4.95</td>
<td>0.54</td>
</tr>
</tbody>
</table>

### Table 3.4: Control variable: $Q$ (thermal activation energy). Equilibrium temperature start, using the parameters for our ‘hot’ thermal regime for all runs.

<table>
<thead>
<tr>
<th>Run</th>
<th>$H$ (µW/m²)</th>
<th>$q_m$ (mW/m²)</th>
<th>$k$ (W/m/K)</th>
<th>$Q$ (kJ/mol)</th>
<th>$A$ (MPa⁻¹)</th>
<th>$q_c$ (mW/m²)</th>
<th>$\tau_{20}$ (Ma)</th>
<th>K:D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>66</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>3.15</td>
<td>0.55</td>
</tr>
<tr>
<td>Q2</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>87</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>6.15</td>
<td>0.16</td>
</tr>
<tr>
<td>Q3</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>108</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>11.3</td>
<td>0.05</td>
</tr>
<tr>
<td>Q4</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>130</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>23.2</td>
<td>0.08</td>
</tr>
<tr>
<td>Q5</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>140</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>34.05</td>
<td>0.08</td>
</tr>
<tr>
<td>Q6</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>150</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>51.68</td>
<td>0.10</td>
</tr>
<tr>
<td>Q7</td>
<td>10</td>
<td>40</td>
<td>2.4</td>
<td>180</td>
<td>$6.30 \times 10^{-7}$</td>
<td>190</td>
<td>198+</td>
<td>NA</td>
</tr>
</tbody>
</table>
### Chapter 3. Results: Morphology and Overturn Time

#### Table 3.5: Control variable: $A$ (viscosity scaling term). Equilibrium temperature start, using the parameters for our 'hot' thermal regime for all runs.

<table>
<thead>
<tr>
<th>Run</th>
<th>$H$ (µW/m²)</th>
<th>$q_m$ (mW/m²)</th>
<th>$k$ (W/m/K)</th>
<th>$Q$ (kJ/mol)</th>
<th>$A$ ($MPa^{-n}$)</th>
<th>$\tau_{20}$ (Ma)</th>
<th>$\Delta$D</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1</td>
<td>100</td>
<td>66</td>
<td>6.30 × 10⁻⁸</td>
<td>66</td>
<td>$13.75 × 10⁻⁷$</td>
<td>6.6</td>
<td>NA</td>
</tr>
<tr>
<td>L2</td>
<td>60</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
</tr>
<tr>
<td>L3</td>
<td>54</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
</tr>
<tr>
<td>L4</td>
<td>50</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
</tr>
<tr>
<td>L5</td>
<td>40</td>
<td>25</td>
<td>2.7</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
</tr>
</tbody>
</table>

#### Table 3.6: Control variable: $\lambda$ (sinusoidal interface wavelength). Equilibrium temperature start, using the parameters for our 'intermediate' thermal regime for all runs.

<table>
<thead>
<tr>
<th>Run</th>
<th>$A$ (km)</th>
<th>$H$ (µW/m²)</th>
<th>$q_m$ (mW/m²)</th>
<th>$k$ (W/m/K)</th>
<th>$Q$ (kJ/mol)</th>
<th>$A$ ($MPa^{-n}$)</th>
<th>$\tau_{20}$ (Ma)</th>
<th>$\Delta$D</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1</td>
<td>100</td>
<td>2.7</td>
<td>66</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>L2</td>
<td>60</td>
<td>2.7</td>
<td>66</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>L3</td>
<td>54</td>
<td>2.7</td>
<td>66</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>L4</td>
<td>50</td>
<td>2.7</td>
<td>66</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>L5</td>
<td>40</td>
<td>2.7</td>
<td>66</td>
<td>66</td>
<td>$6.30 × 10⁻⁸$</td>
<td>2.7</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>
of the volcanic pile into the keel.

For these conservatively low thermal inputs, diapiric overturn occurs in $\sim 10 \, Ma$, comparable to the growth rates of modern marine diapiric core complexes (Martinez et al., 2001). In addition, a large portion of the volcanic pile is returned to the bottom of the crust (here, artificially imposed at 20 km depth).

Another important observation is that after a period of ‘incubation’ where the geotherm evolves from the initial to the equilibrium state (which in this case is not reached before the overturn), a low-viscosity boundary layer forms at the base of the volcanic sequence, and is almost entirely advected into the keel. We marked this with a line in Figure 3.3 A and B, but could not include it in C because the mesh became too fine and the calculation failed. The narrow width of the boundary layer is a direct consequence of the temperature-dependent and non-linear rheology. This is important as much of the komatiitic material is found in the lowermost parts of greenstone stratigraphic sequences, and will therefore be preferentially transported to the lower crust.

### 3.2.2 Simple Parameterizations

We can derive simple parameterizations between $\tau_{20}$ and activation energy $Q$ and temperature $T$. These will form the basis of the scaling relationships we find from our modeling results in the following two sections.

From dimensional analysis we have

$$
\tau_{20} \approx \frac{L}{v} \quad (3.3)
$$

where $L$ is a characteristic depth and $v$ is velocity. $v$ is defined by the relationship

$$
\eta \nabla^2 v \sim \frac{\eta v}{L^2} \approx g \Delta \rho \quad (3.4)
$$

where $\rho$ is density, giving

$$
v \approx \frac{g \Delta \rho L^2}{\eta} \quad (3.5)
$$

Therefore,

$$
\tau_{20} \approx \frac{\eta}{g \Delta \rho L} \quad (3.6)
$$
Approximating the Arrhenius relationship for viscosity as

$$\eta = \eta_0 e^{Q/RT}$$  \hspace{1cm} (3.7)

gives the relationship

$$\tau_{20} \approx \frac{\eta_0}{g\Delta\rho L} e^{Q/RT}$$  \hspace{1cm} (3.8)

The temperature in the upper layer is given by

$$T(y) = T_s + \frac{q_m + HD}{k} y$$  \hspace{1cm} (3.9)

where $T_s$ is the temperature at the surface (which is 273 K in our case) (see Equation 13.13 of Appendix A). Thus

$$\tau_{20} \approx \frac{\eta_0}{g\Delta\rho L} \exp\left(\frac{(Q/R)}{T_s + \frac{q_m + HD}{k} y}\right)$$  \hspace{1cm} (3.10)

We simplify this relationship to isolate the control parameters $Q$ and $H$:

$$\tau_{20} = \alpha \exp\left(\frac{Q}{\mu + \gamma H}\right)$$  \hspace{1cm} (3.11)

where

$$\alpha = \frac{\eta^*}{g\Delta\rho^* L^*}$$  \hspace{1cm} (3.12)

and

$$\mu = R(T_s + \frac{q_m}{k})$$  \hspace{1cm} (3.13)

and

$$\gamma = \frac{RDy}{k}$$  \hspace{1cm} (3.14)

Here, * indicates a reference or scaling value. Choosing reference values of $\eta^* \sim 5 \times 10^{20} Pas$ (an average value for the upper layer), and $\Delta\rho^* = 200 kg/m^3$ gives $\alpha \sim 0.5 Ma$. We can expect our values of $\tau_{20}$ to scale with $H$ and $Q$ in the way described by Equation 3.11.

It should be noted that this scaling applies to the instability amplification time. In fact, $\tau_{20}$ also includes the time to heat up the system, before the instability can begin to grow. In other words,
\[
\tau_{20} \approx \tau_{\text{heating}} + \alpha \exp\left(\frac{Q}{\mu + \gamma H}\right)
\]

Thus, scaling of our model runs must be adjusted to take this into account. In practice, this is not trivial, as for most runs the heating time and the instability growth time overlap. This is particularly true for the fastest models (i.e. when internal heating \( H \) is high or the upper layer has a low activation energy \( Q \)).

### 3.2.3 Changes in thermal regime

We tested the effect of thermal regime on \( \tau_{20} \) and \( K : D \) by systematically varying internal heat productivity \( H \) in the granitic layer as well as heat flow from the mantle \( q_m \). Mantle heat flow had a small effect on the outcomes relative to the effect of varying \( H \); in other words, the primary control on overturn time is the burial of heat-producing elements.

Based on the relationship given in Equation 3.11, we show the effect of varying \( H \) (plotted as \( 1/(\mu+\gamma H) \)) on \( \tau_{20} \) for models H2c-H9c (marked by black dots) in Figure 3.4A. In this suite of models we kept \( q_m \) fixed and increased internal heating from \( H = 3 \, \mu W/m^3 \) to \( H = 10 \, \mu W/m^3 \). This reduced overturn time \( \tau_{20} \) from \( 1067 \, Ma \) to \( \sim 8 \, Ma \).

To fit our data to the parameterizations developed above for this suite of models, we use \( y = 10 \, km \) (the depth of the top layer), \( D = 15 \, km \) (the vertical extent of the heat-producing layer), and the given values of \( k \) and \( q_m \) for this set of models (2.7 \( W/m/K \) and 25 \( mW/m2 \), respectively) in our definitions of \( \mu \) (Equation 3.13) and \( \gamma \) (Equation 3.14).

The scaling law Equation 3.11 then gives

\[
\tau_{20} = 0.4657e^{21905/H}
\]

This fit agrees well with our expected scaling value of \( \alpha \), and suggests a reference value for \( Q^* \) of \( \sim 22 \, kJ/mol \). This is a factor of 3 less than we would expect (given an activation energy of serpentinite of \( Q = 66 \, kJ/mol \)). This should be corrected by subtracting \( \tau_{\text{heating}} \) (Equation 3.15) from \( \tau_{20} \). However, as expected, in most cases there was no clear definition of \( \tau_{\text{heating}} \) since the model overturned as it was still heating. Similarly, growth
Figure 3.4: Variations in internal heating and rheological parameters.
amplification time did not have a clear start as it varies with temperature. This was evidenced by the fact that the granite-greenstone interface reached higher temperatures before it began to deform for models with shorter $\tau_{20}$, even though the viscosity law was the same for all models in this suite (i.e. the interface reached 336° C before deformation initiated when $\tau_{20} = 8.9 \text{ Ma}$ whereas it reached only 293° C before deformation initiated when $\tau_{20} = 65.3 \text{ Ma}$). This suggests that $\tau_{\text{heating}}$ and $\tau_{20}$ overlap in a complex manner.

Nevertheless, we adjusted the fit by defining $\tau_{\text{heating}}$ through visual inspection, by subtracting from $\tau_{20}$ the time at which the sinusoidal interface began to deform. Using this method we were able to compute $Q^* = 45.7 \text{ kJ/mol}$. Given the difficulty in defining $\tau_{\text{heating}}$, this fit appears satisfactory.

We also note that as $\tau_{20}$ becomes greater than $\sim 30 \text{ Ma}$ (the timescale for thermal diffusion), changes in viscosity (and therefore overturn time) are no longer dominated by rising temperatures, but by redistribution of heat by material advection and localized variations in stress.

In contrast, varying $H$ has no effect on the advection of material to the lower crust, indicated by the lack of correlation between $H$ and $K : D$ (marked by black squares). We speculate that $K : D$ is controlled by the viscosity contrast between the upper and middle layers. In cases where the upper layer is rheologically weak, it is able to flow easily downwards. Thus, since changing the thermal regime affects both layers equally at the interface between the two layers, changing $H$ leaves $K : D$ unaffected, and resulting in models which looked much like Figure 3.3.

### 3.2.4 Changes in rheology

The purpose of changing the rheology was to see whether increasing the viscosity from that of serpentinite to that of unaltered basalt would prevent diapirism. Changes in rheology were tested by varying either the activation energy $Q$ (models Q1 to Q7) or the scaling term $A$ (models A1 to A5). Since $Q$ appears in the exponential term, small changes affect the rheology to a much greater extent than small changes in $A$. Thus we use $Q$ as the control parameter for our parametrization of $\tau_{20}$ with rheology, and $A$ as the control parameter to examine the morphological effect of changes in rheology.
Figure 3.4B shows the dependence of $\tau_{20}$ on $Q$ (marked by black dots). It shows that more heat, and therefore a longer ‘incubation’ period, was needed to activate creep for higher values of $Q$. Thus $\tau_{20}$ shows a strong dependence on $Q$, which is the dominant variable in $\eta$ as defined by Equation 3.11. We find a good fit to

$$\tau_{20} = 0.35 e^{0.0327Q}$$  \tag{3.17}$$

Again, this agrees rather well with the scaling value of $\alpha$. As for the scaling obtained between $\tau_{20}$ and $H$ above, however, the exponential factor falls short of the expected value. The values defining $1/(\mu + \gamma H)$ in this suite of models ($y = 10 \text{ km}, D = 15 \text{ km}, q_m = 40 \text{ mW/m}^2, k = 2.4 \text{ W/m/K}$ and $H = 10 \mu \text{ W/m}^3$) predict an exponential factor $\sim 3.5$ times higher than this. In this suite of models, the thermal inputs and therefore $\tau_{\text{heating}}$ is kept constant. Once again, however, $\tau_{\text{heating}}$ was longer than the shortest $\tau_{20}$, and we could not fit the scaling law perfectly. However, by subtracting $\tau_{\text{heating}} = 3 \text{ Ma}$ from $\tau_{20}$ (roughly the time when the temperature at the granite-greenstone interface began to level off for these thermal inputs), we could fit the data to a value of $1/(\mu + \gamma H)$ to within a factor of $\sim 1.7$.

Pushing our models to activation energies approaching those of unaltered basalt was found to be both computationally difficult (such runs could take weeks), and not interesting, since $\tau_{20}$ quickly ran into 100s of millions to billions of years. Clearly, such conditions would make crustal diapirism an unimportant tectonic process. In addition, since greenstones are predominantly hydrously altered (from ultramafic rocks to serpentinite or from basaltic rocks to greenstone), such high activation energies are probably not realistic. This is confirmed by the observed delay between deposition of greenstones and appearance of granites of $20 - 40 \text{ Ma}$ in the mid- to late Archean (Rey et al., 2003).

In contrast to the previous section, however, increasing the viscosity of the upper layer strongly decreases $K : D$. In fact, the effect is so dramatic that small changes in $Q$ quickly make the keel so narrow that it cannot be measured. It also causes Thermax2d to adopt such a fine mesh to delineate the keel that these models do not succeed much past $\tau_{20}$.

Therefore, in Figure 3.5 we show the effect of varying the scaling term $A$ on the
Figure 3.5: Effect of rheology on morphology of the dome-and-keel system. Black lines represent the interface between the upper mafic and middle felsic subdomains plotted at time $\tau_{20}$ when the keel reaches 20 km depth, each labeled with the value of $\tau_{20}$ for that run, as well as an estimate of the viscosity ratio at the interface. Since the viscosity of both layers varies continuously with changing temperature and stress, the viscosity ratio is calculated by taking the ratio of viscosities 2 km away from each side of the boundary, at the time when the interface begins to deform. Four different models are plotted, each having a value of the scaling term $A$ 10 times smaller than the previous mode. The dark dotted line labeled with $0 \, Ma$ represents the initial interface for all models, and the dotted grey line represents the final configuration for a model which does not include elasticity.
morphology of the system. Each black line represents the interface between the upper and middle layers for models A2 to A5 (along with the initial interface shown as a dotted line), and is labeled with the value of $\tau_{20}$ for that model run, as well as an estimate of the viscosity ratio at the interface at the time when overturn was initiated. Note that models A2 to A5 were run using our ‘hot’ thermal regime. As the viscosity ratio is decreased (by reducing the value of the scaling term $A$ by a factor of 10), the keel becomes increasingly narrow, in addition to taking longer to form. This is because as the upper layer rheology is increased, the height of the active boundary layer which flows into the keel decreases.

Hence, the efficiency of crustal reorganization by diapirism is proportional to the weakness (i.e. the degree of hydrothermal alteration) of the volcanic sequence. This may explain the wide range of $K : D$ found in nature, where small variations in effective viscosity would have important morphological effects. Differing levels of erosion and the pinching off of the keel at different depths would also effect surface observations of K:D.

This is an important observation, because it shows not only is diapirism too slow when basalt is left unaltered, it is also inefficient at returning volcanics to the lower crust. Thus, when continents began to rise above sea level, where hydrothermal alteration would have been greatly decreased, diapirism became not only slow, but also inefficient at reorganizing the crust.

### 3.2.5 Changes in model width

We tested the effect of varying the wavelength of the initial perturbation from 40 to 100 km (models L1-L5). We confirmed that for an altered volcanic sequence and intermediate thermal parameters, the fastest growth rate is for model widths of $\sim 50 \text{ km}$ (e.g. de Bremond d’Ars et al. (1999)), and observed a difference in $\tau_{20}$ of $\sim 20\%$ for the other wavelengths tested.

### 3.2.6 The effect of elasticity

We tested the effect of removing elasticity for a number of our models. The main effect was to introduce fine structures (outlined in gray in Figure 3.5), whereas elasticity tends
to dampen these out. It should be noted that the surface doming observed in our models are also observed in salt diapirs. Removing elasticity also increased $\tau_{20}$ by $\sim 10\%$.

### 3.3 Conclusions

For conservatively low thermal inputs ($H = 7 \mu W/m^3$ and $q_m = 25 mW/m^2$) and a hydrously altered mafic upper layer, diapiric overturn occurs in $\sim 10$ Ma. Even for quite cold thermal parameters ($H = 3 \mu W/m^3$ and $q_m = 35 mW/m^2$), diapiric overturn occurs in $\sim 100$ Ma. For $H = 10 \mu W/m^3$ and $q_m = 40 mW/m^2$, which are plausible in the early Archean, overturn can occur in as little as 3 Ma. Moreover, diapiric overturn can recycle important volumes of wet mafic material to the lower crust, with the bulk of the keel consisting of material from the lowest layers of the volcanic sequence (Figure 3.3). In the process, any traces of earlier dome-and-keel formations are erased, and the bulk of komatiitic volcanism sags to the lower crust.

The depth of our dome-and-keel structures is arbitrarily limited to 20 km by the presence of a stiff lower layer, implying that in the absence of such a layer, greenstone belts could extend further. Geophysical data, on the other hand, suggests that GSBs extend to a maximum depth of 10–12 km but are more typically 5–6 km deep (Peschler et al., 2004; Nitescu et al., 2006), which means keels would have reached a maximum of 15–20 km depth before erosion. The vertical structure of GSBs is difficult to resolve seismically, therefore estimates of the depth extent of GSBs has relied heavily on gravity models, which cannot provide unique solutions. Nevertheless, our models can easily be reconciled with such shallow GSBs. First, it is not difficult to imagine that, due to local heterogeneities, complex internal rheologies, and increases in viscosity due to loss of metamorphic water, some natural diapirs would only partially overturn, resulting in an under-developed keel (e.g. Collins et al. (1998)). Second, except for those with small K:D, our model GSBs almost always pinch off at a depth of 10–15 km. Thus, in the case of a complete overturn, the bottom portion of the keel would contribute to and increase the ductility of the lower crust, and leave a remnant upper portion of 15–20 km depth. These sunken tabular bodies of mafic upper crust detached from their keel precursors
(see Figure 3.3) would reorganize the crust leaving the upper crust felsic and the lower crust mafic (consistent with seismic refraction studies), and may perhaps also be the source the numerous sub-horizontal reflectors found in the lower crust (e.g. Rudnick & Fountarin (1995)). In the process, they would have aided ductile horizontal flow in the lower crust, helping mold the remarkably flat Moho characteristic of Archean crust (e.g. James et al. (2003)).

Our models are purposefully simple in design, and are intended to give an upper bound on $\tau_{20}$. Neglected effects are likely to yield even shorter times if included. For instance, if felsic plutons intrude mafic volcanics, or realistic Archean ocean temperatures are used, decreased seawater cooling increases the heat budget and accelerates overturn. Increasing the density of the volcanic sequence with decreasing alteration, the inclusion of brittle deformation, a full 3-dimensional treatment, and dome amplification by melt intrusion would all tend to decrease $\tau_{20}$. Finally, while the secular decrease in temperature makes diapirism more difficult, it is still possible if aided by sporadic thermal events (Rey et al., 2003), thicker volcanic sequences (Ayres & Thurston, 1985), or buckle folding due to far-field horizontal stresses (Cruden & Schrank, 2008).

In summary, our results suggest that crustal diapirism could have been a dominant form of tectonism from the Hadean to the late Archean, when it may have co-existed with an early system of plate tectonics (Lin, 2005). In fact, it seems difficult to avoid diapirism under early Archean conditions in the presence mafic volcanism and a stratified crust (Kamber, 2007). The decrease in thermal inputs and increase in supracrustal viscosity accompanying terrestrial cooling and the rise of continents above sea level eventually impeded crustal overturns of this nature.
Chapter 4

Results: Strain in Crustal Diapirs

4.1 Introduction

Strain is one of the few quantitative structural measurements available for distinguishing between diapiric and other GGT formation processes. Interpretations of observed strains rely on comparisons with analogue and numerical experiments. However, models are difficult to compare with field data because the rheologies used in laboratory and numerical experiments can only approximate the complex rheologies of real geologic terrains, even for simple geometries.

It is nevertheless informative to show how the inclusion of elasticity and stress-dependent rheologies affect the final strain distribution in a simple diapiric overturn. This type of strain analysis constrains deformation processes and adds to the geometric, morphological, and temporal constraint presented earlier.

The quantitative values of strain calculated by our numerical models are limited by numerical diffusion. We will illustrate this effect by testing the same configuration for different mesh sizes. It should be kept in mind, therefore, that our strain values are a minimum value, especially for stress-dependent rheologies or models with narrow shear zones. In addition, the limitations of a plane strain model should be kept in mind when compared with radial dome structures in particular.
4.2 Previous work

The application of predicted strain patterns to granite-greenstone terrains has relied on experimental and analytical solutions for Rayleigh-Taylor or Stokes-type flows (e.g. Ramberg (1967); Dixon (1975); Cruden (1988, 1990); Weinberg & Podladchikov (1995)), and in models aimed at testing diapirism specifically for GGTs (e.g. the centrifuge models of Dixon & Summers (1983), and the numerical models of Mareschal & West (1980)). We will focus on the last two sets of models as we often seen them used in conceptual field-based models of GGTs, and their starting models are comparable to ours. Using simple rheologies and geometries of classic Rayleigh-Taylor theory, Dixon & Summers (1983) and Mareschal & West (1980) have been able to reproduce the broad geometric and kinematic features as well as strain patterns associated with many granite greenstone belts.

In some cratons, comparisons of strains and fabrics across domes and/or the keels with models provide support for the diapir hypothesis (Superior Province: Schwerdtner (1982); Lin et al. (2005); Parmenter et al. (2006); Dharwar Craton: Bouhallier et al. (1995); Chardon et al. (1996); Pilbara Craton: Collins et al. (1998); Van Kranendonk et al. (2004)). However, even in these locations, certain diapir-like strain patterns co-exist with features that are not expected of diapiric structures (e.g. Bouhallier et al. (1995)), and in detail, analysis of complex, heterogeneous granitic domes have caused some authors to reconsider their positions (e.g. Schwerdtner (1984, 1989); Hudleston & Schwerdtner (1997)). In other GGTs, structural analysis has been even less conclusive, providing decades of lively debate (e.g. Barberton: vertical tectonics/diapirism (Van Kranendonk et al., 2009; Anhaeusser et al., 1969) vs. thrust/accretion (Anhaeusser (2006); de Wit et al. (1992) - see Figure 2 of de Wit et al. (1992) for an interpretation of a GSB as a fold and thrust belt).

4.2.1 Dixon & Summers (1983)

Dixon & Summers (1983) were principally interested in the strain distribution in the greenstone keel, although Dixon (1975) also measures dome strain. Their models were
Figure 4.1: Results of the centrifuge modeling of the 2-layered system of Dixon & Summers (1983), shown at an early stage of evolution (Dixon & Summers (1983), Figure 8).
Figure 4.2: Details of the downwards sagging keel from a model similar to that shown in Figure 4.1, but at a later stage in the evolution (Dixon & Summers (1983), Figure 9).
performed in a centrifuge apparatus at strain rates of $10^{-4} - 10^{-5}s^{-1}$ using silicone putty (which has a power-law rheology ($n = 7$) at these strain rates), using a density contrast of 1.07:1, and no temperature dependence. They based their choice of materials on the observation by Schwerdtner et al. (1979) that no ductility contrast existed between greenstone cover and gneissic basement, thus the models had the same rheology throughout. They performed two sets of experiments, one with a simple two-layer model much like ours, and the other intended to investigate the effect of layered volcanic and sedimentary piles in the supracrustal sequence by using a system of layered materials of varying competency. Although this second set of experiments will not be discussed in detail, an important result of these layered experiments was the highly folded and faulted nature of the layered sequences, especially in the upper stratigraphic sections of the keel. In both sets of experiments they were able to reproduce features that could be interpreted as folds and reverse faults.

In their two-layered models, they find that strain in the keels ‘behaved almost like an extensible conveyor belt, rolling into the subsiding trough off the flanking domes and producing strong vertical extension within a narrow band of material trapped within the pinched core of the resulting down fold’ (see Figures 4.1 and 4.2). In particular, they note that in the early stages of development, the axes of maximum strain at the base of the greenstone cover point towards the axis of the keel, a strain pattern which is likely to be overprinted when it sinks further (Figure 4.1). They also note the extreme vertical extension in the center of the keel, reaching up to the surface (Figure 4.2). In contrast, their second set of experiments, strain tended to focus at the keel margins, which they attribute to strain-softening.

In detail, the lack of viscosity contrast between the two layers is probably unrealistic, if only because such a configuration would not result in the observed wavelength of dome and keel structures (see Chapter 2). The measurements of Schwerdtner et al. (1979) which informed their choice in this regard were based on similar directions and magnitudes of strain observed in tonalite-granodiorite dome boundaries, metavolcanic xenoliths, and adjacent greenstone bodies, which were considered to have formed during solid-state diapirism. These narrow contact areas of intense deformation and mixing
are unlikely to be representative of the ductility contrasts in the system as a whole for a number of reasons discussed below. However, since Dixon & Summers (1983) were primarily interested in keel strain, the lack in viscosity contrast across the granite-greenstone interface may not significantly affect their conclusions.

The major limitations of these model results is the lack of temperature dependence. This meant that in the two-layered system deformation was distributed throughout the upper sequence, instead of being focused in a rather narrow (hot) basal boundary at the base of the sequence. This is seen most clearly in the large strains measured at the surface over the keel, where rocks of any composition at $\sim 0^\circ C$ should be more or less immobile.

4.2.2 Mareschal & West (1980)

The details of the Mareschal & West (1980) models have been discussed in Chapters 2 and 3. Although they modeled temperature-dependent rather than stress-dependent rheologies, their strain results are qualitatively similar to those of Dixon & Summers (1983) (Figure 4.3). In addition, they were able to show a reduction in strain towards the upper surface, and a contrast in strain across the granite-greenstone interface. However, this contrast is small (whereas it should be large for the expected viscosity contrast at this boundary) and the distribution of strain in the keel is fairly homogeneous. These limitations are probably due to the use of a single rheology throughout the model, as well as the narrow range of viscosities and the coarse mesh imposed by their numerical limitations.

These two sets of models have remained the standard predictors of strain for diapirism in Archean GGTs (e.g. Parmenter et al. (2006), Collins et al. (1998) (see their Figures 6 and 7), Van Kranendonk et al. (2004)).

4.3 Therma2d Results

We developed a suite of models to test the effect of purely viscous vs. viscoelastic and Newtonian vs. Non-Newtonian rheologies on strain. In addition, we tested the effect of
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**Figure 4.3: Strain pattern predictions from one of the models of Mareschal & West (1980) (Figure 8).**

**Fig. 8.** The accumulated strain at 118 Ma. The maximum strain is 0.5.

Figure 4.3: Strain pattern predictions from one of the models of Mareschal & West (1980) (Figure 8).
mesh size, since we suspected the results of Mareschal & West (1980) may have missed both qualitative and quantitative features of diapiric strain due to coarse resolution. Indeed, we found a number of differences between our models and those described above.

All models presented in this section use the rheological parameters of serpentinite, except for the Newtonian model where we set all stress exponents to 1. The temperature inputs were those of our ‘intermediate’ thermal profile. For most plots, we plot the maximum value of linear strain $\varepsilon_1$, where

$$\varepsilon_1 = \frac{\Delta l}{l} - 1 = S - 1 \quad (4.1)$$

is the fractional difference between the un-deformed and deformed long axis of a strain ellipse, and $S$ is stretch. A more standard strain plot is to plot $S$ for the long and short axes of the strain ellipse (see Figures 4.1, 4.2). We chose to plot $\varepsilon_1$ instead because Thermax2d only allowed for one of the axes of the strain ellipse to be plotted, and since $\varepsilon_1$ falls to zero in unstrained areas, plots of $\varepsilon_1$ are easier to interpret than plots of $S$. For details on our strain calculations, see Appendix B.

4.3.1 Strain Evolution

Keel Strain

We follow the evolution of strain in the case of a visco-elastic, Non-Newtonian rheology (Figure 4.4). We note a number of key features from this figure (where colour plots the magnitude and the white lines show the direction of $\varepsilon_1$), which were not observed in the models of Dixon & Summers (1983) and Mareschal & West (1980):

- Strain is highly localized at the granite-greenstone (GG) interface. This is largely because of the large gradient in viscosity at the bottom of the upper layer due to the model’s strong temperature dependent viscosity. In other words, most deformation occurs in a hot and mobile boundary layer at the base of the greenstone volcanics (cf. Chapter 3.2). This is confirmed in field observations of high-strain zones (HSZ’s) in the greenstone at the granite-greenstone contact, which can be between 200 m to 2 km wide (Parmenter et al., 2006).
Figure 4.4: This plot shows the evolution of strain during a diapiric overturn. Plotted in colour is $\varepsilon_1 = \Delta l/l - 1$ (see colour bar for scale and Appendix 1 for details) for a model run which included both elasticity and stress-dependent viscosity. The direction of $\varepsilon_1$ is shown by the white lines. Note that while the colour scale is kept constant in all frames, the length of the lines are proportional within frame, but have no relation to the length of the lines in either of the other frames.
• Strain down the axis of the keel can be of the same order as that at the GG interface, depending on what stage of the evolution of the keel is being observed. In general, however, it is less, contrary to the predictions of Mareschal & West (1980) and the two-layered models of Dixon & Summers (1983).

• There is a zone between the GG interface and the axis of the keel which undergoes very little strain. The width of this zone depends on the depth and stage of evolution which is being observed. For instance, assuming 10 km of erosion as before, this relatively un-deformed zone would appear much wider in outcrop at the stage shown in Figure 4.4B than in Figure 4.4C. Furthermore, if we could resolve realistically narrow zones of strain, this un-deformed area would be larger still. It should be noted that, if examined carefully, there is a hint of this un-deformed area in the models of Dixon & Summers (1983) despite the restricted range of viscosities.

• In detail, principal directions of strain in the narrow strain zone at the granite-greenstone interface are not straightforward (see also Figure 4.10). In our models, this is likely due to numerical noise in this highly strained zone. However, the inhomogeneities found in nature should produce even more complex strain patterns in these highly strained areas, and at the strain rates implied by our quickly descending keel (a keel evolving from 10 to 20 km in 1 Ma gives strain rates of \( \sim 6 \times 10^{-14} \) s\(^{-1}\), which is on the high end of reasonable tectonic strain rates).

**Dome strain**

Little strain is recorded in our model domes, even at the granite-greenstone interface, contrary to the models of Dixon & Summers (1983) and Mareschal & West (1980). Strain in the dome is almost entirely limited to the lowest parts at a late stage of overturn evolution. For our granitic rheology, the temperatures and low stresses at the top of the dome result in viscosities reaching our upper limit (\(10^{28} \) Pas, see Chapter 3, Figure 3.3). In contrast, the older models had highly restricted viscosity contrasts, or no contrast at all at the granite-greenstone interface.

However, our lack of dome strain follows the trend observed by Dixon (1975), who
performed centrifuge models of diapiric structures using domes with either higher or lower viscosities than the overburden. He found lower dome strain in the first case (which he compared to gneiss domes), and higher strains in the second (which he compared to salt domes). He also notes that the viscosity contrast between real gneiss domes and their overburden was likely greater than the one used in his experiments (where the dome was \( \sim 4.3 \) times more viscous than the overburden), implying even less strain in the domes than he was able to measure.

There is, of course, strain observed in real GGT batholiths, and it is typically much more complex than that of the associated greenstone keels (e.g. Schwerdtner (1982); Chardon et al. (1996); Collins et al. (1998); Van Kranendonk et al. (2004)). For example, ‘typical granitoid complexes are ... aggregates of smaller structures, notably oval gneiss
domes or doubly plunging folds and oval to crescentic plutons’ or ‘unstrained plutons cut the pattern of gneissosity, but this may mean only that the rise of the plutons outlasted the gneiss doming’ Schwerdtner (1989) (Figure 4.5). Hence, Schwerdtner (1989) recognizes first- and second-order structures within broadly domical granitic batholiths. Importantly, although real batholiths exist with a variety of internal complexity (see Mount Edgar dome vs. the chaotic Shaw Dome, Pilbara craton (Collins et al., 1998; Van Kranendonk et al., 2004)), in general their complex interiors are in contrast to their simple outlines (Van Kranendonk et al., 2004).

Unlike our model batholiths, batholith strain closely matches greenstones strain where the two subdomains meet, suggesting little ductility contrast at the contact (see Chapter 4.2, Van Kranendonk et al. (2004)). We attribute this to the fact that, in detail, GGT contacts are complex, with greenstone xenoliths in the granite, felsic ‘strips’ in the greenstone, and late-stage plutons focused at the contact (e.g. Schwerdtner et al. (1979); Schwerdtner (1989); Collins et al. (1998)). These heterogeneities may reflect complicated intrusion processes at the time of formation of the granite body which most likely predated doming (Chapter 1.1.2, Cruden & Robin (1998)). For instance, Collins et al. (1998) interpret the Mount Edgar Batholith (Pilbara Craton) to have formed as intrusive sheets during doming, which continued after keel formation ended, a process which undoubtedly complicated the rheology of the batholith as a whole, and particularly at the edges. Moreover, high-strain shear zones are likely to channel metamorphic water from below, hydrating and altering the rheology of the contact rocks. Considering these and other effects, the rheological properties of the domes towards the contacts are expected to differ from that of our homogeneous quartz-diabase.

Nevertheless, our models suggest that deformation in the interiors of batholith resulting from any form of solid-state diapirism should be minimal except near the base of a late-stage keel. Strain patterns within domes, then, either predate doming (Schwerdtner (1989)), or are a result of the complicated emplacement of, remelting of, or intrusion into granitoid complexes. These processes are secondary to diapiric doming, although they may occur before, during, or after diapirism, or be triggered by doming. Our models and the complexity of real granitic domes suggest that these secondary processes deform the
bulk of the dome more than diapirism itself. This is probably not true at the contact with
the volcanic cover sequence where complex intrusive events and metamorphic alterations
lower the viscosity of the granitic material; however, we do not capture those effects in
our models. Nevertheless, it appears difficult to use strain in the cores of GGT batholiths
to determine if the large-scale dome-and-keel structure was formed by diapirism. This is
reinforced by the fact that these complex internal structures tend to be bound by domical
shapes which are consistent with diapirism.

In the final stages of the evolution, strain in the granite at the tip of the keel is
extreme (here, reaching values of up to 20), perhaps contributing to the gneissosity of
the lower crust.

4.3.2 The effect of Mesh Size

The computational cost of these numerical models limit both the magnitude of strain
and the resolution of the zones of high strain. Our main goal here is to see what details
of the strain distribution are hidden in models with coarse gridding. For these models,
the mesh size was constrained at the onset of the run. If necessary for the solution to
converge, however, Thermax2d did refine the mesh in certain areas (e.g. Figure 4.7B). In
the unconstrained case, Thermax2d was allowed to optimize mesh size on its own from
the beginning.

Figure 4.6 compares results for different meshes, and Figure 4.7 plots the meshes used
in each case. Qualitatively, we can see that the 5 km mesh smears out strain (Figure
4.6B,E), concealing first-order features such as the shear zone at the granite-greenstone
interface. When left to its own devices, however, Thermax2d reproduces the qualitative
features of the finer mesh quite well, losing only $\sim 20\%$ of the strain magnitude (Figure
4.6C,F). Both the 5 km and unconstrained cases tend to exaggerate strain below the
sagging keel and above the rising dome. In addition, decreasing mesh size causes a slight
increase in overturn time.

As predicted, the magnitude of strain when the mesh is 1 km is up to a factor of
2 greater than in the other two cases. Hence we caution that the magnitudes of strain
calculated in our models are merely useful in comparison to each other, and should not
Figure 4.6: Three models run at different mesh sizes, shown here at time $\tau_{20}$ and at a more evolved stage. All models are visco-elastic and Non-newtonian. The mesh sizes were: A: 1 km; B: 5 km; and C: unconstrained (see Figure 4.7).
Figure 4.7: Here we show the mesh for the three models runs in Figure 4.6, in the more evolved state.
be compared with real continuum processes.

### 4.3.3 The effect of stress dependence and elasticity

![Graph showing strain in crustal diapirs](image)

**Figure 4.8:** This plot summarizes the effects of model rheologies on strain at time $\tau_{20}$. The magnitude of $\varepsilon_1$ is shown in colour (here, A-D each have their own scale) and its direction is shown by the white lines. Mesh size for all 4 models was constrained at 1 km.
Figure 4.9: This figure shows the value of strain along the midline of the descending keel at $\tau_{20}$, for four different rheologies. Red lines are for models including elasticity, blue are for purely viscous models; solid lines are stress-dependent viscosities, dashed lines are for stress independent viscosities.

Figure 4.8 summarizes the effect of rheology on strain patterns. In addition, we plot the magnitude of strain down the axis of the keel (Figure 4.9) and at the granite-greenstone interface (Figure 4.10), measured at time $\tau_{20}$ when the keel has reached 20 km depth. Based on these three plots we note that:

- Visco-elasticity and Newtonian rheology both tend to increase the magnitude of strain in the keel axis with respect to that at the granite-greenstone interface, and to reduce the area of the strain-free zone in the keel. Presumably, this is because these both act to de-localize strain, spreading deformation throughout the keel.

- At this stage in the evolution, elasticity has little effect on the morphology (although it plays an important role in filtering small-wavelength features at later stages), but does slightly decrease overturn time (cf. Chapter 3.2.4). Newtonian rheologies also lengthen overturn time, because deformation must be accommodated by a wider area.
Figure 4.10: This figure shows the value of strain along the greenstone-granite interface at $\tau_{20}$, for four different rheologies. Lines are notated in the same manner as in Figure 4.9.

- For non-Newtonian viscosities, elasticity appears to increase the magnitude of strain in localized areas. This effect is not noted for Newtonian viscosities.

- As mentioned above, strain at the granite-greenstone interface is highly complex, exhibiting significant short-wavelength variability. We believe this is an a computational effect, as this area of high shear is most susceptible to numerical noise. However, the overall structure and the relative magnitudes are still evident.

- Overall strain in the viscous, non-Newtonian case (measured as $\int \varepsilon_1 dA / \int dA$ where $A$ is the area of the upper domain) is $\sim 2/3$ that of the overall strain in other models. We speculate that this is because models with viscous, non-Newtonian rheology should exhibit the narrowest shear zones in our suite of models, and our 1-km resolution is insufficient in this case. Nevertheless, when considered alone, this model displays an even greater redistribution of strain away from the keel midline and towards the granite-greenstone interface, as would be expected for models with
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strong shear localization.

- Area is not always conserved due to numerical error, hence in some places \( \varepsilon_1 < 0 \).

In summary, the combined effects of elasticity and non-Newtonian rheology result in differences in strain magnitude of approximately a factor of 2. Of the two, non-Newtonian rheology has the greatest effect.

### 4.4 Magnitude of strain

It has been suggested that the magnitude of strain observed in greenstone belts is too low when compared with strain measured in diapir experiments (A. Cruden, personal communication). Indeed, a major motivation for the work presented in this chapter was to see if elasticity or non-Newtonian rheology or a combination of these could account for Dr. Cruden’s impression that GGT strains are too low to be explained by diapirism.

Magnitude of the total geological strain is often described by

\[
e_s = (\sqrt{3}/2) \gamma_0
\]

a variation of the natural octahedral unit shear

\[
\gamma_0 = \frac{2}{3}[(E_1 - E_2)^2 + (E_2 - E_3)^2 + (E_3 - E_1)^2]^{1/2}
\]

where \( E_1 = \ln(1 + \varepsilon_1) \) (Hossack, 1967). The models of Dixon & Summers (1983) attain values of up to \( e_s \sim 2.5 \). In our plane strain models \( \varepsilon_1 = -\varepsilon_3 \) (in principle), therefore \( \gamma_0 = \frac{2\sqrt{6}}{3} \ln(1 + \varepsilon_1) \) and \( e_s = \sqrt{2} \ln(1 + \varepsilon_1) \). We attain maximum values of \( e_s \sim 3 - 4.5 \) in the later stages of keel formation (i.e. after \( \tau_{20} \)) for models with a 1 km mesh (Figure 4.11). In contrast, Mareschal & West (1980) calculate strains of only 0.5-0.6 at a similar stage (see Figure 4.3).

A limited number of average strains and individual measurements in greenstone belts around the world are summarized in Hudleston & Schwerdtner (1997) (Table 3.4.1) and Condie (1981). They range from 0.41 to 3, lower than but compatible with our calculated magnitudes. However, axial ratios of > 1:1:50 have been recorded elsewhere.
Figure 4.11: Plot showing the natural octahedral strain $e_s$ (defined in Equations 4.2 and 4.3) for a model which is visco-elastic and non-Newtonian. Colour represents the magnitude $e_s$ and the black lines represent its direction.

(Collins et al., 1998), and stretch values of 20 to 100 are noted at granite-greenstone contacts (Figure 4.12, S. Lin, personal communication). Indeed, Hudleston & Schwerdtner (1997) point out that the measured averages they present may not be representative.
of the regional strain, due to sampling bias (rocks must contain strain markers, which tend to be the coarser-grained and more competent rocks; highly metamorphosed rocks are preferentially eroded; and strain markers are lost in zones of very high strain). In addition, strain may not have been measured at the granite-greenstone contact (S. Lin, personal communication).

Figure 4.12: A: Un-deformed pillow basalts from the Carrot River Greenstone Belt (Superior Craton) Lin (2005). B: Strained pillows from the same belt, where the pillows are still recognizable; C: Mylonite, which S. Lin believes to have also been pillows, but whose primary structures have been destroyed under high strain conditions (S. Lin, personal communication).

As it turns out, then, both the numerical modeling and field measurements underesti-
mate strain. Thus, although we have cautioned against comparing our numerical values against true continuum processes, these numbers suggest that strain magnitude in greenstone belts are similar to those seen in both analogue and numerical models. Indeed, if we were able to reproduce a 200 m wide high-strain zone (Parmenter et al., 2006) instead of our 1 km wide one, our strains would approach those observed ($\varepsilon_1 \sim 50 - 100$).

4.5 Conclusion

Our models predict strain in general agreement with those of Dixon & Summers (1983) and Mareschal & West (1980). Some important differences are the development of highly localized shear zones at the granite-greenstone interface, the relatively un-deformed zone between the granite-greenstone interface and the axis of the keel, and almost no strain near the surface and in the granitic dome (Figure 4.4). The effect of visco-elasticity vs. viscosity on the magnitude or principal direction of strain did not significantly affect strain in our models, although perhaps it would have if we were able to run them at higher resolution. More important was the inclusion of non-Newtonian and temperature-dependent rheology, which focused strain in narrow high strain zones, as are observed in granite-greenstone contact areas (e.g. Lin et al. (2005); Parmenter et al. (2006)). Finally, although our numerical calculations are limited by mesh size, the magnitude of strain our models produce are comparable to the limited number of magnitude estimates quoted in the literature, which, as it turns out, probably also underestimate strain magnitude.

Strain patterns predicted by our simple models are clearly to be used only as a general guide, particularly in the case of batholiths which retain complex pre- and post-diapirism structures and perhaps a limited record of diapirism itself away from the margins. The soft rheology and high strains of greenstone keels tend to erase heterogeneities, and our models have perhaps more predictive value in these regions. In addition, it has been suggested that GGT rocks display Newtonian instead of non-Newtonian behaviour in some areas (P.-Y. Robin, personal communication). Therefore, strain in GGTs may resemble the models of Dixon & Summers (1983), Mareschal & West (1980), the ones presented here, or a combination of them.
On the other hand, highly complex rock assemblages will inevitably deform in ways that may, at the outcrop scale, be contrary to the general sense of strain in the GGT as a whole. This may be particularly true at the granite-greenstone interface.

Unfortunately, in most cases, geological strain measurements are subject to a variety of differing interpretations, and have not been able to resolve the diapiric vs. horizontal tectonics for granite-greenstone terrains. Our hope is that the strain patterns and evolution obtained from our models may help resolve this issue. However, the issue is undoubtedly complicated by the complexity and magnitude of the geologic record, which we cannot hope to reproduce, and disagreement about the timing of events. Moreover, some of the confusion may stem from comparisons of events that occurred at different times in the evolution of granite-greenstone terrains. As we have shown, active diapiric overturn and dome-and-keel emplacement after the initial incubation period can occur in a very short time (< 1 Ma), shorter than the typical resolution of U-Pb dating. Thus it is difficult to determine whether intrusions or other deformation structures pre- or post-date the formation of these or other first-order features of the dominant tectonics. In addition, granitic intrusions internal to greenstone belts may need to be considered differently from those defining the boundaries of the greenstone belts (Jelsma, 1993); internal batholiths are likely to pre- or post-date diapirism, and the resulting strain patterns may not reveal much about the rapid evolution of dome-and-keel structures.

Future strain modeling with Thermax2d should include: stratifying the upper layer as did Dixon & Summers (1983); including inner domes or tabular bodies in the granitic middle layer, such as are observed; and, if possible, running models with a smaller mesh.
Chapter 5

Geochemical implications

Having quantified the modeling results, we investigated the implications of diapirically emplacing large volumes of wet metavolcanics in the lower crust. In particular, sinking mafic volcanics into the lower crust may have important implications for the formation of the large volumes of tonalite-trondhjemite-granodiorite (TTG) which dominate Archean terrains but whose origins are unclear. In addition, melting of wet metavolcanics in the lower crust leaves a restite which must have either passed through or contributed to the budding sub-cratonic lithospheric mantle (SCLM).

To test whether the return of wet ultramafic metabasalts to the base of the crust by diapirism could melt to form TTG we performed a suite of geochemical calculations using the program MELTS (Ghiorso & Sack, 1995). These were not intended to be a full geochemical treatment of the problem, but were aimed at testing our model to see if further geochemical work might be warranted.

5.1 Geochemical constraints: a brief overview

Although there remains much debate about the formation of or even the classification of TTGs (they span a broad range of geochemistries (Moyen & Stevens, 2006)), analyses of field samples as well as high-pressure melting experiments provide constraints for our equilibrium melting experiments. Archean SCLM is even more enigmatic, and is constrained mainly by seismics and analysis of mantle xenoliths (which probably suffer
from a sampling bias). In addition, both field analyses and experiments are often strongly
guided by a preferred tectonic model, making the published literature quite difficult to
navigate.

5.1.1 Geochemistry of TTGs

TTGs are siliceous ($SiO_2$ between 65 and 70 wt %), aluminous ($Al_2O_3 > 15 \%$) rocks,
and constitute up to two-thirds of Archean crust (Moyen & Stevens, 2006). They are
distinguished by their sodic nature and (K/Na below 0.4) and their strongly depleted
heavy rare earth elements (HREE). HREE depletion is quantified as the ratio of the
concentration of a light REE to a heavy one, typically La/Yb. For TTG, La/Yb is on
average 38.4, but can reach up to 150. In addition, unlike modern granites, TTG do
not typically show a Europium anomaly, indicating a lack of plagioclase in the residue
(Moyen & Stevens, 2006).

TTGs are thought to result from partial melting of hydrated metabasalts (eclogite
or amphibolite facies) in the garnet stability field (e.g. Smithies & Champion (2000)),
from a source rock derived from the mantle less than 150 Ma before melting (Moyen &
Stevens, 2006). As a strong fractionator of heavy rare-earth elements (HREE), garnet is
needed to explain TTG’s characteristic HREE-depleted geochemical signature. Garnet is
stable at 8-15 kbar and $700 - 1000^\circ C$, or at 15-25 kbar and $700 - 900^\circ C$, implying TTG
formation at the base of an over-thickened crust in the first case, or by slab melting in the
second (Moyen & Stevens, 2006), with garnet as an important component in the residue.

A thickened crust may have formed by magmatic underplating; however, it is unclear
how this mechanism would have provided the necessary hydration. Slab melting is rare
in modern tectonics, but may have been more common in the Archean (e.g. Martin et al.
(2005); Lee (2006)) if the mantle was significantly hotter.

TTG are generally Fe and Mg poor, and have have Mg # ($Mg/(Mg+Fe)$) between
30 and 40 (Martin et al., 2005; Moyen & Stevens, 2006). There is an evolution in Mg #
from low to high from the early to the late Archean, as well as an increase in average
$SiO_2$, which has been interpreted by supporters of horizontal tectonics in the Archean as
an increasing interacting of slab melts with the mantle wedge as the angle of subduction
increased through the Archean. In addition, TTG have a strong resemblance with modern adakites, rare sodic rocks generally linked to slab melting at anomalously hot subduction zones (Martin et al., 2005; Moyen & Stevens, 2006). However, TTGs older than ~3.3 Ga have low MgO# and Cr and Ni concentrations, indicating little interaction with the mantle wedge (Martin et al., 2005; Moyen et al., 2007).

If, as our models show, wet metabasalts can be returned to the lower crust by diapirism, subduction or magmatic underplating may not be required to form TTGs (e.g. Bédard (2006)). A number of studies present results of high-P,T experiments deriving TTG-like melts from a small range of starting compositions (see Moyen & Stevens (2006) for a compilation). These experiments have not been conclusive, and there remains much debate about whether melting at 8-15 kbar and 700-1000 C, or at 15-25 kbar and 700-900 was the likely mechanism. They all suggest, however, that the restite of melting to form TTG is garnet-rich and therefore likely to be too dense to remain in the SCLM, ultimately returning to the mantle instead.

However, relatively few source compositions (especially ultramafic or komatiitic) have been tested. Our model calculations show that if komatiitic volcanism were present, a considerable proportion of it would be preferentially deported to the lower crust. Moreover, thermal models of the mantle predict that Archean and pre-Archean oceanic volcanism may have been significantly more komatiitic than preserved terrains suggest (Nisbet & Fowler, 1983). Not all observed GSBs contain komatiite (Ayres & Thurston, 1985); however, as our modeling shows, altered komatiite, if it is the lowest layer and also has the lowest viscosity in the sequence, will have been hidden by diapirism, making the source regions for TTGs at the base of a thickened crust more komatiite-rich than has been assumed. Thus, it is interesting to test whether a starting composition rich in komatiite could produce a TTG-like melt under the conditions outlined above.

5.1.2 Geochemistry of the SCLM

The Archean SCLM is characterized by its relative strength and its net neutral buoyancy. That is, its positive chemical buoyancy offsets the negative thermal buoyancy at every depth (Cooper et al., 2006; Lee, 2006), known as the isopycnic hypothesis (Jordan, 1988).
Analysis of mantle xenoliths reveal that Archean SCLM tends to have a highly depleted upper layer, and a less depleted but still distinctively Archean lower layer (O'Reilly et al., 2001). Moreover, Re-Os isotopic studies of xenoliths indicate that Archean SCLM is approximately the same age as the overlying crust (Lee, 2006), although some suggest that the age recorded by the SCLM corresponds only to the last tectono-magmatic activity in the area (Carlson et al., 2005). In addition, while it may contain areas of high garnet concentration (making these areas denser than the average SCLM), the SCLM as a whole probably contains less than 1% garnet (Carlson et al., 2005). Its unusual geochemical and physical properties has protected the SCLM (and Archean terrains) during multiple Wilson cycles, and was formed by a process which extracted 30-50% melt from its mantle source (Lee, 2006).

The formation of Archean SCLM has been variously attributed to one of three end-member scenarios (Lee, 2006), each of which has some limitations: i) the restite of a melt-depleted mantle plume; ii) horizontal and vertical stacking of oceanic lithospheres during repeated subduction; or iii) arc-related accretion and thickening.

To produce 30-50% partial melt, the plume hypothesis calls upon a single hot (>1650°C) mantle plume which remains active for the history of the craton, which may span up to 700 Ma (Van Kranendonk et al., 2004). In addition, the degree of melting would vary from the hottest to the coldest part of the plume, resulting in a gradation in fertility of the residue. While large, hot plumes are plausible in the Archean, the SCLM (as sampled by mantle xenoliths) shows no evidence of such zoning (O'Reilly et al., 2001; Lee, 2006). Furthermore, the plume hypothesis does not account for the fact that much of the SCLM appears to have originated at lower pressures before being transported to its present depth (Carlson et al., 2005; Lee, 2006).

The second hypothesis requires a thicker, more buoyant oceanic crust than today’s to avoid being subducted after cooling; even then, the dense eclogitic base would have to be removed before accretion (Carlson et al., 2005; Lee, 2006). Moreover, this model implies that SCLM accumulation was episodic, and predicts a systematic variation in SCLM composition, as would be seen in a stack of imbricated modern oceanic lithosphere (Lee, 2006). Neither of these predictions are supported by age dating and geochemistry of
mantle xenoliths (Lee, 2006).

The third scenario invokes the accretion of lithosphere underlying island arcs in a subduction environment (Lee, 2006). Since terrane boundaries appear to extend into the lithospheric mantle (O’Reilly et al., 2001), it is difficult to explain the SCLM which is underlying terrains such as the Pilbara, which is devoid of elongated features or transcending faults (Van Kranendonk et al., 2004), using the arc-accretion model. Finally, the last two scenarios both make the uniformitarian assumption that strong plates dominated tectonic processes, which is mechanically questionable during the Meso-Archean and especially the Hadean (see Chapter 1).

Alternative models have recently been proposed to avoid these difficulties, notably the catalytic delamination model of Bédard (2006). Bédard (2006) proposes that instead of the complex series of slab windows, break offs, and fortuitously-placed plumes called on to explain the geology of many terrains in the Superior Province, a much simpler vertical tectonic scenario would be just as effective and more realistic. Moreover, a simple mass balance calculation suggests that the volume of melt required to form large Archean terrains is incompatible with slab melting. He performed a series of geochemical equilibrium models and showed that the TTG-type rocks of the Minto Block (Superior) could be the result of in-situ two-stage melting of wet metabasalt. His final model, in broadest terms, is that repeated cycles of plume activity provide mafic and ultramafic inputs to the crust whose partial melts form TTGs, and whose restites delaminate and descend through or mix with depleted plume residues, instigating further mantle melting. Our thermo-mechanical modeling provides a mechanical context for his model. Unlike his model, however, we propose that not all the restite would descend through the mantle.

5.2 Geochemical modeling

Using the thermodynamic model MELTS 2.0 (Ghiorso & Sack, 1995), we explored the possibility of forming TTG by partial melt of increasingly ultramafic wet metabasalt. Our aim was to produce melts that had HREE patterns (represented in spider diagrams) typical of TTGs, as well as modal composition and density of restite (a mixture of garnet,
olivine, and ortho- and clinopyroxene (O’Reilly et al., 2001; Lee, 2006)), for reasonable temperatures and melt fractions. In particular we were interested in creating TTG-like melts that left a residue with some garnet, but with a density less than 3.32 g/cm³ (the density of Archean SCLM at the base of the crust (O’Reilly et al., 2001)).

5.2.1 MELTS 2.0

MELTS 2.0 is a publicly available program that calculates thermodynamic equilibrium of phases in magmatic systems. It takes as input a starting composition and a pressure and temperature, calculates the equilibrium compositions of the solids and melts, and outputs tables containing the composition and thermodynamic properties of the resulting melts and residues. MELTS can execute a series of such calculations as a function of a chosen parameter.

Once a starting composition is entered, MELTS allows a number of different approaches to running equilibrium geochemical calculations. For each execution, there is a choice of mode: isobaric, isothermic, isenthalpic, isentropic, isochoric, geothermal, or PTpath. For example, we could fix the pressure, and execute a series of equilibrium calculations over a range of temperatures, giving different percentages of melts and compositions. Or, given a fixed percentage of melt, we could run calculations over a range of pressures, giving different temperatures and melt/restite compositions. Each calculation outputs a series of files containing basic physical properties (densities of the liquid and the restite, viscosity, $fO_2$, etc), trace elements of the liquid and the residue, modal compositions of the residue, etc., for each incremented variable. MELTS uses partition coefficients from McKenzie & O’Nions (1991), and offers the option of normalizing the trace element output using the primitive mantle values of Sun & McDonough (1989).

Unfortunately, the Ghiorso & Sack (1995) found after the publication of the first version of MELTS that a factor of 3 in the expression for the logarithm of the activity coefficients for garnet was missing. The faulty formula is the default. They offer the option of a fix for this problem; however, it is not fully integrated in the calculation and may result in inaccuracies in other parts, such as melt fraction or modal abundances. Since garnet is such an important part of our system (both for its effect on the melt
Chapter 5. Geochemical implications

HREE and on the density of the restite), we opted to use the garnet fix. Resulting effects on other parts of the system could not be tracked.

We fixed the oxygen fugacity for all calculations using the FMQ buffer (i.e. where the oxygen fugacity as a function of temperature and pressure is maintained by the redox buffer fayalite-magnetite-quartz). The presence of these minerals controls the oxidation state of Fe, and therefore has an important effect on the relative proportions of mineral assemblages. Together with the magnetite-wustite (MW) and hematite-magnetite (HM) buffers, the FMQ covers most of the fugacities found in the crust and upper mantle, and it has been shown that most igneous rocks are formed under fugacities near the FMQ buffer (Carmichael & Ghiorso, 1986).

Execution of each set of calculations was quite rapid - a few minutes at most. Most calculations failed or never started, as each initial composition had only a narrow range of equilibrium P,T conditions under which they were possible, which were unknown a priori. As a result, much time was spent ‘tweaking’ initial parameters, ranges of calculations, and ‘step-sizes’.

5.2.2 Results

Preliminary tests were done using mixtures of typical or average komatiite and basalt compositions (trace and major elements) from different cratons available in the literature (e.g. Jochum et al. (1991); Sproule et al. (2002) and Jayananda et al. (2008) as well as ‘average’ compositions taken from Condie (2005)). Specifically, we systematically tested mixtures ranging from 20% komatiite and 80 % basalt to 80% komatiite and 20% basalt, taking the same proportions for all components of the starting compositions.

Using the isobaric mode, we found that TTG-like melts could be produced for compositions with up to ∼40% komatiite at a variety of depths (8 – 20 kbar, or 30 – 70 km depth). At pressures <∼ 8 kbar garnet is not stable (e.g. Lee (2006)). Higher proportions of komatiite in the mixture was too Mg-rich and SiO$_2$ poor, leaving the melt too mafic to be TTG-like. However, the melts and residues were highly variable, depending on mostly on initial composition, which can be quite different from one terrain to another, as well as water content and initial conditions. This seemed rather adhoc, and this methodology
The results presented here (Figures 5.1 and 5.2) are for calculations following a melt fraction contour (15 or 20 %), at 8 kbar and 15 kbar and with 1% water. We include in these starting compositions for basalt (Jochum et al., 1991), mixtures of basalt and komatiite (whose unmixed compositions were taken from Jochum et al. (1991)), sample compositions from mafic dykes syntectonically placed into TTGs (Condie, 2002), and komatiitic basalt (Malviya et al., 2006). We compared the resulting melts to average TTGs from field samples and from experiments (Martin et al., 2005). Note that not all published analyses include the same trace elements, making comparisons somewhat difficult.

We were not able to produce a melt whose spider diagram precisely matched those of an average TTG. Since we were starting with real measured geochemistries, and there probably doesn’t really exist an ‘average’ TTG, this is hardly surprising. In some cases, we were able to closely approximate the REE pattern of experimental TTGs. We note that not all published compositions include the same set of REE; thus, in Figure 5.1, the spider diagrams of observed average TTG (black squares) and average experimentally derived TTG (black circles) appear to be incomplete with respect to our MELTS modeling results.

The main result of our geochemical models is that, under the same experimental conditions, melts show increasingly better fits to observed and experimental TTG with increasing komatiite content in the starting composition - better even than komatiitic basalts or mafic dykes (Figure 5.1). As stated previously, at more than 40% komatiite, it is difficult to melt out enough SiO$_2$ in a single melting event. However, it is possible that two-stage melting would produce the required compositions, since the secondary melt would be higher in SiO$_2$.

Elemental compositions in Figure 5.2 refer to the composition of the melt. Our SiO$_2$ and Al$_2$O$_3$ generally fall close to those of the average TTG, as do the La/Yb and K/Na ratios (although these last are variable, as indeed they are in nature). However, our Mg and Fe content as well as our Mg# are low compared to the average, as well as to the expected range. Once again, however, the best fit for these values are for a starting
composition of 40% komatiite.

Density of the restite is variable (Figure 5.2). At 8 kbar (a depth of \( \sim 25 \text{ km} \)), most starting compositions except the most mafic ones may leave a restite which is less than or similar to the density of the SCLM at the same depth. If melted at 15 kbar (requiring higher melt fractions), the restite is much denser than the SCLM. This suggests that some TTG formation systems will leave a restite which could remain in the SCLM, while other systems would leave a restite destined to sink through the SCLM.

5.3 Conclusion

The results of our models are that, under the same conditions, melting of a komatiite-rich source composition (up to 40% komatiite) replicates measured TTG properties better than other tested compositions. This suggests that, given the huge range of geochemical and geophysical settings which must have given rise to TTG magmas, similar results could be achieved through a more rigorous analysis. At the very least, our results indicate that the diapiric descent of wet metabasalts with considerable volumes of komatiite may have been an important part of TTG petrogenesis and the Archean continent formation story, and warrants further study.

The fate of the restite of this melting must be to either descend through the SCLM, or to contribute to it. Bédard (2006) endorses a model for vertical tectonics in the Minto Block of the Superior Province where most granitic rocks are formed by partial melting of the lower crust. He performed extensive geochemical equilibrium calculations using source rocks from field observations to support his theory, and argues that the restite of melting of metabasalts at the base of the crust, which is garnet and clinopyroxene rich, and therefore dense, should descend through the SCLM, thereby enriching it on its way through and catalyze further melting. His and other melting experiments, as well as our own, indicate that the density of the restite of melting metabasalt is such that only under limited mechanical and geochemical conditions will this restite contribute directly to the SCLM. Another alternative, however, is multiple stage melting of komatiite to eventually form granitic rocks, which should leave a restite which is essentially dunitic, and therefore
Figure 5.1: *Geochemical modeling:* We compare the REE and major element properties of our komatiite/basalt melts with average TTG properties. Here, 2kom8bas refers to the mixture of komatiite and basalt used (in this case, 20% komatiite mixed with 80% basalt). Starting compositions are discussed in the text. Note that the greater the proportion of komatiite in the mix, the better the fit to the observed and experimental average TTG compositions. All models were run with 1 wt% H2O, and in the presence of the FMQ $fO_2$ buffer.
Figure 5.2: Summary of our results. Starting compositions are labeled as in Figure 5.1, and are described in the text. Garnet (wt%) refers to the amount of garnet in the restite. All other components listed refer to the composition of the melt.
less dense, which could contribute directly to the SCLM by vertical accumulation.

Thus, in the case of SCLM formation by vertical accumulation, the ultra-depleted upper portions of the SCLM would have been formed by material which was first partially melted out of the mantle as mafic to ultramafic volcanism, then returned to the lower crust where it was partially melted again at least once to form the continental crust. Such a two-stage process may be a more efficient mechanism for reaching the 30-50% fractional melting required by mantle xenolith composition than 1-stage melting in a plume or oceanic lithosphere. In addition, this model accounts for evidence indicating that much of the SCLM formed at shallow depths before being transported downwards. Moreover, rapid diapiric overturn rates such as our models suggest would allow for the formation of the SCLM to closely follow and be coupled to the formation of the continental crust.
Chapter 6

Summary and Discussion

Archean cratons represent the culmination of earlier Hadean tectonics. They are set apart from Proterozoic cratons by the presence of granite-greenstone belts, by the abundance of chemically unique tonalite-trondhjemite-granodiorite granitoids (Moyen & Stevens, 2006), and by the presence of unusually strong and depleted (30-50% partial melts) sub-continental lithospheric mantle (O’Reilly et al., 2001; Carlson et al., 2005; Lee, 2006). Age dating shows that these features unique to Archean crust typically form in sequence: voluminous cycles of ultramafic to mafic volcanics (relics of which now form the greenstone keels of GSBs) are followed closely (within $\sim 40 \, Ma$) by the appearance of granitic domes (Rey et al., 2003), while the sub-cratonic lithosphere forms roughly simultaneously with (and is coupled to) the crust (Bédard, 2006; Lee, 2006; O’Reilly et al., 2001; Rey et al., 2003; Carlson et al., 2005). While their relative timing suggests they are genetically linked, currently popular mechanisms for the formation of GSBs, TTG, and the SCLM appear difficult to integrate into a single tectonic context. Our thermo-mechanical models of crustal diapirism, however, may provide a basis for reconciling all three processes.

6.1 Summary

The visco-elastic models presented in Chapters 2-5 show that crustal diapirism under Archean conditions reproduce structures compatible with much of what is known of granite-greenstone belts. In addition, they show that in the hotter conditions of the
Hadean and early Archean, diapirism would have been a rapid and efficient crustal recycling mechanism. Indeed, given the evidence for a compositionally stratified crust and subaqueous volcanics up to 4.4 Ga, diapirism appears difficult to avoid. In the process, significant volumes of the hydrated volcanic sequence would have been displaced to the lower crust, where they would be available for remelting to form TTGs. In particular, komatiitic volcanism in the lower portions of the volcanic sequence would be preferentially deposited there.

Strain mapping of our numerical crustal diapirs, while limited by numerical diffusion, closely matches observed strain in greenstone belts, which is also underestimated by biased sampling and lack of markers in the most highly strained regions. This lends further support for the hypothesis that GGTs formed by diapirism, and may help determine Archean tectonic processes from field observations. Our results also suggest that internal deformation in the infamous gregarious batholiths (MacGregor, 1951) of GGTs may not be diagnostic of the primary tectonic mechanism.

Melting at the base of the crust has been one of two possibilities for the formation of TTGs; however, a physical mechanism to keep the lower crust well supplied with wet metabasalts has been lacking. Our small suite of geochemical calculations suggest that volcanics returned to the base of the crust may provide the source for melting to form TTGs. Moreover, we suggest that melting of komatiite-rich lower crust may be a good alternative, and warrants further investigation.

6.2 Discussion

The results of our modeling lend support to the vertical tectonic hypothesis (e.g. MacGregor (1951); West (1980); Goodwin (1981); Ayres & Thurston (1985); Collins et al. (1998); Van Kranendonk et al. (2004)) for the in-situ generation of cratonic continental crust and subcontinental cratonic mantle, in the following form (Figure 6.1). Vigorous Hadean volcanism rapidly built thick piles of hydrously altered mafic to ultramafic volcanics. When their thicknesses reached a few tens of kilometers (which may have taken significantly less than 100 Ma if Archean rates (Ayres & Thurston (1985)) are taken as
a lower limit), heating at the base, aided by the the release of metamorphic fluids from the hydrated volcanics, began to generate felsic melts (Kamber et al., 2005). Subsequent mafic volcanics atop these felsic layers would have rapidly found their way back to the base of this nascent felsic crust by diapirism, as early as \( \sim 25 \) Ma after extraction from the mantle. This process continued to fuel the generation of the felsic crust, churning the lower crust into the gneissic state we see preserved today as Archean basement.

Aided by the release of water from the hydrous phases, one or two-stage melting of young metabasalts at lower crustal depths generated rocks with the bulk composition, rare earth element and isotope signatures of Archean TTGs, while the depleted harzburgitic restite would have remained largely dry, strong, and garnet-bearing (although by no means homogeneous). The restite thus contributed to the SCLM in one of two possible scenarios. In the first, the dense restite of metabasaltic melting delaminated and traversed or mixed with mantle plume restites à la Bédard (2006). Alternatively, the formation of TTGs by one- or two-stage melting of mixed mafic and ultramafic volcanics left a lighter (dunitic) restite, contributing to the growth of the SCLM by vertical accumulation from above.

A simple mass-balance calculation shows that a 30 km thick TTG-dominated crust over a 200 km thick harzburgitic SCLM can be achieved by 15% partial melt of 230 km of ultramafic volcanics returned diapirically (with 100% efficiency) to the lower crust. For the rates of volcanism of more than 1 km/Ma which are seen in the late Archean (Ayres & Thurston, 1985), this can be accomplished in 200 to 250 Ma, and presumably faster in the Hadean. This mass balance requires much melting from the mantle, and, since a significant fraction of the volcanics remains at the surface, poses problems for removing the remainder by erosion. However, as pointed out by Bédard (2006), mass balance is a problem for many models of Archean crustal growth (see Chapter 5.1.2).

A key point here is that less mafic metabasalts will leave a restite too rich in garnet to form the chemically buoyant SCLM (due to their abundant supply of garnet-forming constituents); greater proportions of komatiitic volcanism than are preserved (Arndt & Nisbet, 1982; Nisbet & Fowler, 1983) or selective removal of komatiite to lower crustal levels are required to eventually form the SCLM by top-down accumulation. However,
Figure 6.1: Cartoon of Summary Model. Mafic and ultramafic seafloor volcanism builds a pile which thickens until the bottom melts, creating a felsic upper crust. Further volcanism (1) is hydrously altered and returns diapirically to the lower crust (2). Upon remelting, these (ultra)mafic sequences form TTGs and the bulk of the continental crust (3). At 30-40 km depth, melting of a mafic to ultramafic source leaves a garnet-bearing harzburgitic residue (4), giving the granitoids their HREE-depleted signature. The descent of the (ultra)mafic volcanics to the lower crust would metamorphose the serpentinitic/greenschist volcanics to the amphibolite facies, releasing water and facilitating the re-melting and deformation of surrounding mafic and felsic rock. The restite would be dry, strong, depleted and buoyant relative to the mantle, vertically accumulating at the top of or descending through the growing SCLM (5). The structure of the SCLM and its overlying crust can vary significantly at all scales. Therefore this model predicts neither a homogeneous nor a systematically zoned SCLM, produces TTGs soon after the extraction of their source rock from the mantle, couples the formation of the crust and the SCLM, and does not require strong plates or shallow subduction.
despite its buoyancy, Archean SCLM does contain eclogite, in some areas in significant amounts (O’Reilly et al., 2001; Carlson et al., 2005; Lee, 2006). A top-down model for the formation of the SCLM does not preclude the formation and eventual return to the mantle of eclogitic packages. Indeed, it predicts a crust and SCLM which can be heterogeneous at all scales, and also permits contributions from other mechanisms operating simultaneously. For instance, the restite of plume melting (also probably required for the formation of komatiites) may have contributed the less depleted portions of some SCLM (O’Reilly et al., 2001), which conveniently relieves the mass balance and chemical constraints outlined above.

Subsequent secular cooling of the mantle would have shut down this mechanism, leaving the last stages of the transition frozen as the Archean we see today. Thus, although this model of Hadean continental crust generation requires more elaboration and testing (especially the geochemical implications), our numerical results suggest it a plausible alternative to the plate-tectonic and plume scenarios currently under consideration for the formation of Earth’s early crust and subcontinental lithospheric mantle.

In summary, our thermo-mechanical results (Chapters 2-5) provide a geodynamic context for the redistribution of wet metavolcanics to the Archean lower crust, which is an essential part of any final model for the simultaneous creation of Archean crust and the SCLM by vertical tectonics. When combined with processes such as proposed by Bédard and/or the ones presented in Chapter 5 for generating the correct chemistry of Archean crust and mantle roots, our models provide a link between SCLM formation and surface geology, without invoking mechanically strong plates or shallow subduction, or relying on a series of fortuitous tectonic coincidences.

Archean crust preserves the final failure of diapiric tectonics. Reasons for this failure may include decreasing mantle-derived volcanism associated with secular cooling of the mantle, the secular decay of crustal HPEs, and the reduction of the supracrustal density inversion as felsic volcanics were added along with sediments associated with the elevation of the crust above sea level.
Part II

Venusian Mantle Diapirs
Chapter 7

Introduction

Among the most intriguing classes of topographic features on Venus are approximately 500 quasi-circular coronae (Stofan et al., 1992, 2001; Glaze et al., 2002). These are circular to elliptic volcanic features abundant on the Venusian surface and apparently unique in the solar system. Attributed to short-lived mantle upwellings (thermals), they may play a significant role in cooling the planet (up to 25%) (Johnson & Richards, 2003). However, the dynamics of corona formation are poorly understood.

Venus’s similar size and bulk composition implies that the forces driving tectonics and mantle convection should be similar to those operating on the Earth. However, Venus is devoid of the trenches, rifts and faults characteristic of Earth-like plate tectonics, most likely because its hot and dry surface gives the crust and lithosphere a prohibitively large yield strength (e.g. Solomatov & L.-N.Moresi (1996)). A number of models have been proposed to account for this, for instance the cessation of a plate tectonic regime (Solomatov & L.-N.Moresi, 1996), or episodic overturn events (Turcotte, 1993; Parmentier & Hess, 1992). In addition to these forms of tectonism, however, it is likely that coronae must be an important tectonic process on modern plate-less Venus.

Coronae are typically $\sim 250 \text{ km}$ in diameter (Glaze et al., 2002; Hansen et al., 1997) and are concentrated in a large triangular region bounded by the highlands Atla, Beta and Themis (known as the BAT region) (Figure 7.1a) (Stofan et al., 1992; Johnson & Richards, 2003). Interpretations of the axisymmetric shapes of coronae, combined with their association with a broad variety of volcanic and tectonic features (Stofan
et al., 1992; D.M. Janes, 1992; Smrekar & Stofan, 1997a; Stofan et al., 2005), have contributed to a general picture that they are, directly or indirectly, related to transient upwellings from the upper mantle or the core-mantle boundary (CMB) (e.g. Johnson & Richards (2003); Herrick & Phillips (1992); Schubert et al. (1989); Jurdy & Stefanick (1999); Hansen (2003)), the nature and origin of which remain an area of active research (Johnson & Richards, 2003; Smrekar & Stofan, 1997a; Janes & Squyres, 1995; Koch & Manga, 1996; Hoogenboom & Houseman, 2005; Dombard, 2006; Sandwell & Schubert, 1992; J.E. DeLaughter, 1991). In contrast, the BAT highlands themselves are generally thought to reflect continuous and strong upwelling flow in the mantle. This picture stems from considerations of a combination of large volcanic constructs on each of the highlands (e.g. Smrekar & Stofan (1997a)) as well as strong axisymmetric geoid highs analogous to those observed over Hawaii (Simons et al., 1997).

Johnson & Richards (2003) analyze the statistical distribution of coronae characterized by positive gravity anomalies, plausibly explained by dynamic support from upwelling flow in the mantle. These authors find that whereas the majority of these ‘uncompensated’ features are concentrated within the BAT region, the distribution of compensated coronae is relatively insensitive to geographical region. From the geometric relationship between the BAT highlands and uncompensated BAT coronae, along with inferences drawn from the results of laboratory experiments on mantle convection (e.g. Schaeffer & Manga (2001); Jellinek et al. (2002, 2003a)), Johnson & Richards (2003) develop a conceptual model for a mixed-mode style of Venusian mantle convection that explains the temporal coexistence of coronae and the highlands (Figure 7.1b).

In particular, Johnson & Richards (2003) envision that mantle convection driven by heat transfer from Venus’ core is in a regime characterized by two types of upwelling. Approximately steady flow in long-lived narrow axisymmetric conduits, akin to the style of flow often inferred to occur within mantle plume conduits (i.e. ‘tails’) in the Earth (e.g. Whitehead & Luther (1975); Loper & Stacey (1983); Richards et al. (1989)), gives rise to the highlands (see discussions in Nimmo & McKenzie (1996) and Vezolainen et al. (2003)). In contrast, transient mantle thermals (Turner, 1973; Ogawa et al., 1991; Manga & Weeraratne, 1999) are suggested to explain coronae (Schaeffer & Manga, 2001; Jellinek
et al., 2002).

The Johnson & Richards (2003) model is consistent with available geophysical and volcanological constraints and elegantly explains the coexistence of coronae and the highlands. However, while the model is plausible, the inferred large lateral variations in the style of mantle upwelling flow at the CMB present a difficult conundrum for existing geodynamic models of mantle convection. In particular, long-lived, axisymmetric plume conduits are thought to be characteristic of upwellings that are greater than one or two orders of magnitude less viscous than surrounding mantle (Whitehead & Luther, 1975; Loper & Stacey, 1983; Jellinek & Manga, 2004; Morris & Canright, 1984; Griffiths & Campbell, 1994; Lenardic & Kaula, 1994; Jellinek et al., 2003b; Kerr & Mériaux, 2004), whereas transient thermals are typical of flows in which the viscosity variations are order unity (Jellinek et al., 2002; Olson & Singer, 1985; Manga et al., 2001). In addition, under thermally steady-state conditions a number of studies have implied or shown that the conditions leading to either upwellings in the form of thermals or upwellings in the form of low viscosity plumes are distinct and highly restrictive (Jellinek & Manga, 2004; Hansen & Ebel, 1988; Nataf, 1991) and thus it is unclear how two such regimes may occur together at the same time.

For example, approximately isoviscous thermals are expected to form if the internal mantle temperature is close to that of the core-mantle boundary, a characteristic of stagnant lid convection expected to occur in a one-plate planet (Solomatov & Moresi, 2000; Schubert et al., 2001). In contrast, the large temperature variations in the hot thermal boundary layer that can give rise low viscosity plume conduits may arise only in an active lid regime characterized by subduction and large-scale stirring of the cold lithosphere into the mantle (Jellinek & Manga, 2004; Lenardic & Kaula, 1994; Thayalan et al., 2006).

Thus, to explain the coexistence of uncompensated BAT coronae and the Atla and Beta regions with a mixed-mode model (Figure 7.1b) an essential issue is to establish the origin of large lateral differences in the temperature drop across the thermal boundary layer at the core-mantle boundary of Venus.

An important point is that the spatial and temporal coexistence of thermal regimes
Figure 7.1: a) Corona distribution superposed on a map of the Venus geoid modified from Johnson & Richards (2003). Coronae are concentrated within a triangular area bound by the BetaAtlaThemis (BAT) highland regions (red triangle). Beta and Atla are characterized by strong, axisymmetric positive geoid anomalies, consistent with dynamic support from mantle upwelling. b) A conceptual model for a mixed-mode style of Venusian mantle convection proposed by Johnson & Richards (2003) to explain the coexistence of dynamically-supported coronae (principally within the BAT region) and the highlands themselves. Whereas coronae are proposed to be the surface expression of transient thermals, the highlands are better explained in terms continuous axisymmetric mantle upwellings.
giving rise to contemporaneous low viscosity mantle plumes and isoviscous mantle ther-
mals is problematic if and only if Venus is currently in a thermally steady-state regime. Indeed, it is unclear whether it is reasonable to expect such a condition. Constraints on the mean surface age derived principally from cratering studies (Phillips et al., 1992; Strom et al., 1994; McKinnon et al., 1997) are consistent with an average surface age of only 700-800 Myr. In addition, the results of detailed analyses of the local statistics of cratering populations (Hauck et al., 1998) and recent geological mapping (Stofan et al., 2005; Guest & Stofan, 1999) are collectively consistent with either a rapid (∼ 100 Myr) or more gradual (> 400 Myr) global resurfacing of the planet. Explanations of the nearly uniform and young surface age have been presented in terms of a catastrophic overturn of the Venusian lithosphere followed by little resurfacing thereafter (e.g. Strom et al. (1994); Parmentier & Hess (1992); Schaber et al. (1992); Turcotte (1993); Turcotte et al. (1999)), a more gradual resurfacing (Guest & Stofan, 1999) and the outward expression of an episodic style of plate tectonics (Turcotte, 1993; Turcotte et al., 1999; Moresi & Solomatov, 1998; Solomatov & L.-N.Moresi, 1996).

Although the time scale and style for resurfacing is poorly constrained, the fundamental transition in tectonic regime to a current one-plate state beginning about 700-800 Myr ago remains undisputed. If the resurfacing is related to a foundering of the litho-
sphere occurring on a time scale of 100 - 400 Myr then it is reasonable to hypothesize the Venusian mantle to be currently adjusting to a new thermal condition (e.g. Nimmo & McKenzie (1998)).

Here we present laboratory experiments aimed at exploring in detail the transient regime of mantle convection that may follow an overturn of the lithosphere. We also investigate the transient regime following the cessation of forced large-scale stirring. In addition to characterizing these regimes, our goal is to identify whether it is reasonable to expect such a mixed-mode of convection, as described in Figure 7.1b, in the mantle of Venus following a lithospheric overturn. Our laboratory results are supported by numerical work presented in Robin et al. (2007), which will be described briefly.
Chapter 8

Laboratory Experiments

8.1 Apparatus and Method

Our convection experiments were performed in the $30 \times 33 \times 22.5$ cm tank shown in Figure 8.1. The sidewalls were insulated plexiglass. The upper (cold) and lower (hot) boundaries were aluminum heat exchangers through which cold and hot water was pumped at a high rate, such that isothermal boundary conditions, characteristic of Rayleigh-Bénard convection, were achieved.

Our working fluid was ADM 36/43 corn syrup, which has a viscosity that depends strongly on temperature (Table 8.1). In addition, this corn syrup was particularly clear in colour, which improved our visualization of the flow.

Submerged a few millimeters below the cold boundary was a 2 mm thick motor-controlled ‘conveyor’ belt constructed of reinforced neoprene that was used to drive a tank-filling large-scale flow. The belt was extensively drilled with 1 cm diameter holes to maximize thermal contact with the roof heat exchanger.

At the start of each experiment, boundary temperatures were set such that the system evolved to a regime of steady-state stagnant lid convection at high Rayleigh number that was quantitatively similar to previous studies (e.g. Manga & Weeraratne (1999); Manga et al. (2001)) (Figure 8.1b, Table 8.2). A statistical steady-state was indicated by constant and equal heat fluxes at the cold and hot boundaries and a well-defined mean internal temperature that did not vary in time. The belt was positioned near the top of the
Figure 8.1: a) A schematic diagram of the experimental apparatus. b) Cartoons showing stagnant-lid and (forced) active-lid convection in our experiments.
### Table 8.1: Physical Properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of thermal expansion of syrup*</td>
<td>$\alpha$</td>
<td>$5.6110 \times 10^{-4}{^\circ}C^{-1}$</td>
</tr>
<tr>
<td>Density of syrup*</td>
<td>$\rho$</td>
<td>$\rho(T) = 10^3(-5.6077410^{-4}T + 1.46201)\text{kg/m}^3$</td>
</tr>
<tr>
<td>Dynamic viscosity of syrup**</td>
<td>$\mu$</td>
<td>$\mu(T) = \exp(6.7057 - 0.1353T + 0.0004T^2)\text{Pa s}$</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g$</td>
<td>$9.81\text{m/s}^2$</td>
</tr>
<tr>
<td>Thermal conductivity of syrup*</td>
<td>$K$</td>
<td>$K(T) = 0.365 + 0.00245T\text{W/m}^1\text{C}$</td>
</tr>
<tr>
<td>Thermal diffusivity of syrup**</td>
<td>$\kappa$</td>
<td>$110^{-7}\text{m}^2\text{s}$</td>
</tr>
</tbody>
</table>

* from (Jellinek et al., 2003b). ** measured in the laboratory.
stagnant part of the cold thermal boundary layer and thus does not influence the flow in this regime (Jellinek et al., 2003b).

Once this basic state was established the conveyor belt was turned on at a fixed velocity that we varied. Resultant large-scale flow overturned and stirred the cold thermal boundary layer into the underlying fluid, forcing an active-lid style of convection (Moresi & Solomatov, 1998) (Figure 8.1c). Where possible the belt was driven until thermally steady-state conditions were achieved. However, the large viscous stresses involved in stirring the cold lid into the underlying fluid made the experiments technically difficult, and ultimately limited the range of parameter space we were able to investigate (Table 8.2).

<table>
<thead>
<tr>
<th>Run</th>
<th>Regime</th>
<th>Ra</th>
<th>Pe</th>
<th>$\lambda^*_t$</th>
<th>$\lambda^*_l$</th>
<th>$\theta$</th>
<th>$q^*$ (W/m²)</th>
</tr>
</thead>
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<tr>
<td>14</td>
<td>Stagnant Lid</td>
<td>$5.4 \times 10^7$</td>
<td>-</td>
<td>4</td>
<td>4</td>
<td>0.75</td>
<td>980</td>
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<td>Transient 1</td>
<td>$2.9 \times 10^7$</td>
<td>9100</td>
<td>15</td>
<td>19</td>
<td>0.61</td>
<td>2400</td>
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<tr>
<td></td>
<td>Active Lid</td>
<td>$2 \times 10^7$</td>
<td>9100</td>
<td>11</td>
<td>17</td>
<td>0.6</td>
<td>2000</td>
</tr>
<tr>
<td>15</td>
<td>Stagnant Lid</td>
<td>$5.2 \times 10^7$</td>
<td>-</td>
<td>4</td>
<td>4</td>
<td>0.745</td>
<td>970</td>
</tr>
<tr>
<td></td>
<td>Transient 1</td>
<td>$3 \times 10^7$</td>
<td>23000</td>
<td>12</td>
<td>22</td>
<td>0.66</td>
<td>2000</td>
</tr>
<tr>
<td></td>
<td>Active Lid</td>
<td>$2.6 \times 10^7$</td>
<td>23000</td>
<td>8</td>
<td>19</td>
<td>0.63</td>
<td>1100</td>
</tr>
<tr>
<td>17</td>
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<td>$1.1 \times 10^8$</td>
<td>-</td>
<td>4</td>
<td>5</td>
<td>0.78</td>
<td>1300</td>
</tr>
<tr>
<td></td>
<td>Transient</td>
<td>$8.6 \times 10^7$</td>
<td>4500</td>
<td>8</td>
<td>13</td>
<td>0.75</td>
<td>2900</td>
</tr>
<tr>
<td></td>
<td>Active Lid</td>
<td>$5.7 \times 10^7$</td>
<td>4500</td>
<td>7</td>
<td>12</td>
<td>0.66</td>
<td>2100</td>
</tr>
<tr>
<td>18</td>
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<td>4</td>
<td>4</td>
<td>0.79</td>
<td>1300</td>
</tr>
<tr>
<td></td>
<td>Transient 1</td>
<td>$3.2 \times 10^7$</td>
<td>2300</td>
<td>4</td>
<td>6</td>
<td>-</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>Active Lid</td>
<td>-</td>
<td>2300</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>19</td>
<td>Stagnant Lid</td>
<td>$2.8 \times 10^7$</td>
<td>-</td>
<td>4</td>
<td>4</td>
<td>0.75</td>
<td>1200</td>
</tr>
<tr>
<td></td>
<td>Transient 1</td>
<td>$2.6 \times 10^7$</td>
<td>31000</td>
<td>35</td>
<td>-</td>
<td>-</td>
<td>3300</td>
</tr>
<tr>
<td></td>
<td>Active Lid</td>
<td>-</td>
<td>31000</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 8.2: Description of 5 experiments discussed in the text. All transient flows are complex and properties are based on measurements made at stack 1 and stack 2 (Fig. 8.1). In cases where there are no values reported for the transient or active-lid regimes we could not maintain a fixed velocity condition at the to surface for sufficient time to obtain a reliable measurement. * is the maximum during the transient, and the mean for stagnant- and active-lid. Other values represent means.

Experiments were quantified using time series of temperature and local heat flux. Local heat flux was measured using four Omega HFS4 heat flux sensors distributed across the hot boundary (Figure 8.1). Wire thermocouples were located along the hot,
cold and sidewall boundaries, and in the interior of the system. To characterize the local vertical and lateral temperature and viscosity variations in the hot thermal boundary layer in both transient and steady-state regimes, as well as the corresponding local heat fluxes, we applied thermocouple stacks above two heat flux sensors (referred to as stack 1 and stack 2). Stack 1 and stack 2 are constructed of 4 to 6 J-type thermocouples spaced 0.5 – 1 cm apart, designed to record the downstream evolution of the hot thermal boundary layer occurring in response to the forced spreading cold material. In addition, the qualitative structure of all flows was characterized using a combination of time-lapse and still photographs of shadowgraphs, which capture fluid motions by mapping vertical and lateral variations in refractive index that occur with corresponding changes in temperature.

8.2 Dimensionless Parameters

Five dimensionless parameters characterized our experiments. The aspect ratio, $A = \frac{w}{H} = 1.3$, was constant. All experiments were conducted at high Prandtl number, $(Pr = \frac{\mu}{\rho \kappa} \geq 10^4)$ such that the Reynolds number $(Re = \frac{\rho V L}{\mu})$ for all experiments was less than about unity and inertial effects were neglected. Here, $\mu$ is viscosity, $\rho$ is density, $\kappa$ is thermal diffusivity, $H$ is the layer depth and $w$ is the tank width (Table 8.1). The vigour of buoyancy-driven motions is characterized by the Rayleigh number,

$$Ra = \frac{g \rho \alpha \Delta T H^3}{\mu_i \kappa} \quad (8.1)$$

where $\mu_i$ is the viscosity based on an appropriate mean interior temperature (Table 8.2), $\Delta T$ is the temperature drop from the hot boundary to the cold boundary, $g$ is gravity and $\alpha$ is the coefficient of thermal expansion.

The velocity of the imposed circulation was varied for each experiment and is expressed with a Peclet number,

$$Pe = \frac{V H}{\kappa} \quad (8.2)$$

where $V$ is the belt velocity. This number represents the balance between the rate of advection to the rate of thermal diffusion. For a forced rate of advection, as is the case
here, it determines the relative importance of driving velocities on the structure of the flow (e.g. Richter & Parsons (1975); Lux et al. (1979)). Lux et al. (1979) find that when \( Pe \) exceeds a critical value of \( Pe_{\text{crit}} = 0.2Ra^{0.6} \), the flow becomes dominated by single-cell convection in a \( 4 \times 1 \) aspect ratio box; for a smaller aspect ratio box, the transition would occur for smaller values of \( Pe \), which they do not test. For the three with the fastest imposed belt velocities, \( Pe \) falls well above \( Pe_{\text{crit}} \) as defined by Lux et al. (1979) during the active lid phase of the model run, and the flow is dominated by the belt velocity. For the two models with moderate \( Pe \) during active lid (runs 18 and 19 - see Table 8.2), \( Pe \) is slightly less than \( Pe_{\text{crit}} \) as defined by Lux et al. (1979). However, since in our models the aspect ratio is \( \sim 1 \), \( Pe_{\text{crit}} \) will be less than for the \( 4 \times 1 \) aspect ratio models of Lux et al. (1979); thus for runs 18 and 19, it is not clear whether the flow structure would be dominated by the imposed advective forcing at those belt speeds. However, even if steady-state active could have been achieved (it was not), the small aspect ratio of our system would not have permitted multiple cells to develop in any case.

The magnitude of the total viscosity variations in the system is given by the total viscosity ratio,

\[
\lambda_t = \frac{\mu_c}{\mu_h} \tag{8.3}
\]

where the subscripts \( c \) and \( h \) denote parameters measured at the cold and hot boundaries.

All of our experiments were conducted under approximately constant and high \( Ra \) (\( \geq 10^7 \)) conditions (Table 8.2). In addition, \( \lambda \sim 10^3 \), such that the convection was in the stagnant lid regime when \( Pe = 0 \) (Jellinek et al., 2002; Manga & Weeraratne, 1999).

Along with these external parameters it will be useful to introduce some additional parameters determined internally. We define internal temperature, \( \theta = (T_i - T_c)/(T_h - T_c) \) and the hot boundary layer viscosity ratio, \( \lambda^*_h = \mu^*_i/\mu_h \). Because we are interested in transient phenomena, which may not be global in scale, \( \lambda^*_h \) is a local viscosity ratio, where the superscript * indicates values based on the maximum temperature differences recorded at stack 1 and stack 2. For the same reason, we define a local heat flux ratio \( q^* \), which is the measured convective heat flux, \( q \), normalized to the average steady-state stagnant lid heat flux, \( q_s \). We also define the local internal temperature normalized to the stagnant lid value, \( \theta^*_i = (T^*_i - T_c)/(T^*_i - T_c) \), where the superscript \( s \) denotes 'stagnant
lid’. Under statistically steady-state conditions these local parameters are equivalent to the global values.
Chapter 9

Results

In Table 8.2 we present results from 5 experiments from a larger series of 21 runs. In particular, we identify and characterize two transient thermal regimes. The first (transient 1) occurs when the belt is turned on, and the system is forced to evolve from steady-state stagnant-lid convection towards steady-state convection in the active-lid regime. The second (transient 2) occurs when the belt is turned off, and the system returns from steady-state active-lid convection towards a fully developed stagnant-lid regime. Owing to practical difficulties involved with achieving steady-state active-lid convection over a range of $Pe$ conditions our discussion of this regime is limited to its qualitative features.

9.1 Qualitative results

9.1.1 Transient 1: Stagnant lid to active lid convection

Figures 9.1 and 9.2 are time series of shadowgraph images characterizing the transition away from a stagnant lid regime as the cold boundary layer is stirred into the underlying fluid through one complete overturn. In Figure 9.1a, $Pe = 0$ and the flow is in the stagnant lid regime under statistically steady-state conditions. Convection is in the form of intermittent rising and sinking thermals. The internal temperature, $\theta = 0.76$, and the viscosity ratio, $\lambda_h = 4$ (i.e order 1), which are quantitatively consistent with previous studies (Schaeffer & Manga, 2001; Jellinek et al., 2002; Manga & Weeraratne, 1999;
Figure 9.1: Shadowgraph images showing the evolution of the system away from a stagnant-lid regime following initiation of forced stirring from above. a) Steady-state stagnant-lid convection in which upwellings are transient thermals. Transient cold downwellings are not observed in this image but are apparent in time series of temperature. b) The conveyor belt at the cold boundary is turned on, resulting in a forced advection of the cold stagnant lid down the sidewall to the floor of the tank. c), d) Cold fluid spreads across the floor and is stirred into the fluid interior. $Ra = 1.1 \times 10^8$, $Pe = 4500$, and $\lambda_t \approx 10^3$. 
Manga et al., 2001). The very small refractive index contrast between the upwelling
thermals and colder fluid interior is indicative of the small temperature difference that
corresponds with an order 1 viscosity variation (Jellinek & Manga, 2004; Manga et al.,
2001).

Figures 9.1b-d and 9.2 capture the evolution in flow regime after the belt is turned on.
Cold and dense fluid, characterized by a high refractive index contrast, is forced down
the sidewall and along the hot boundary. Hot thermal boundary layer fluid is, in turn,
overrun and ‘bulldozed’ ahead of this advancing front of cold fluid (e.g. Tan et al. (2002))
resulting in a thermal boundary layer that thickens monotonically downstream. Local
advective thickening of the hot thermal boundary layer directly ahead of the cold front
enhances convective instabilities so that the frequency of thermal formation is higher
than that occurring further downstream (Figure 9.2), where the thermal boundary layer
grows by vertical thermal diffusion alone. The magnitude of this spatial variation in
thermal formation frequency depends on the importance of lateral advection of thermal
boundary layer fluid and consequently increases with $Pe$. This is discussed in more detail
below.

Hot thermal boundary layer that is overrun by the cold current is trapped as a so-
called ‘squeeze layer’ (Snyder & Tait, 1998). Further thickening of the squeeze layer by
conductive heat transfer from the hot boundary leads to convective instabilities that take
the form of low viscosity plumes with large heads and narrow axisymmetric conduit tails
rising through the cold layer (Figure 9.2) (Jellinek & Manga, 2004; Olson & Singer, 1985).
These plume heads are larger in diameter than the thermals forming downstream of the
spreading cold fluid. Where possible the ratio of the diameter of the plume heads to the
diameter of the thermals was measured as close to the leading edge of the hot boundary
layer as possible and found to be proportional to $(l^*_h/\lambda^*_h)^{1/3}$, consistent with expectations
from Rayleigh-Taylor theory (Moresi & Solomatov, 1998; Selig, 1965; Biot & Odé, 1965;
Lister & Kerr, 1998).

An essential characteristic of this transient regime is that large lateral variations in
temperature and viscosity across the hot boundary layer lead to a mixed mode style of
flow characterized by a contemporaneous formation of approximately isoviscous thermals
and low viscosity plumes in the same flow. However, it is important to note that once the cold material blankets the cold boundary entirely the flow from the hot boundary is in the form of low viscosity plumes only. Thus, in our system the coexistence of these two types of upwelling structures is a characteristic of the early part of this transient regime. More generally, the longevity of this regime depends on the rate at which the cold boundary layer is overturned, $Pe$, and the length of the hot boundary expressed as a function of the aspect ratio, $A$, which we do not vary.

### 9.1.2 Transient 2: Active lid to stagnant lid convection

Active lid convection under thermally steady-state conditions is achieved in only a few cases. An essential difference to the stagnant lid regime is that the stronger cooling effect of stirring the cold fluid in contact with the top boundary into the underlying fluid interior leads to a lower interior temperature and to larger temperature and viscosity variations in the hot thermal boundary layer. A time series of shadowgraph images illustrating steady-state active lid convection and the thermal transient following the cessation of the imposed stirring is shown in Figure 9.3. Figure 9.3a shows a fully developed flow composed of an asymmetrical large-scale flow along with sheared low viscosity plumes ascending from the hot boundary (Jellinek et al., 2003b; Gonnerman et al., 2005) (Table 2). Figures 9.3b and 9.3c show the transient regime in which the forced flow has ceased and plumes with large heads rise vertically. Because the interior temperature is less than in the stagnant lid regime, vertically rising plume heads carry a comparatively much greater excess temperatures (indicated in Figure 9.3 by the large contrasts in refractive index compared to Figure 9.1a), and are significantly less viscous and larger than thermals.
Figure 9.2: Shadowgraph showing a snapshot from transient 1. The advancing cold front extends to midway across the tank. Upstream from the cold front, $\lambda_h^* = 60$ and nascent low viscosity plume instabilities (large heads) are observed. Downstream from the cold front $\lambda_h^* = 4$ and upwellings are thermals. The clustering of thermals near the leading edge of the cold front reflects a higher frequency of thermal formation. This is interpreted to occur because the lateral spreading of cold material causes the hot boundary layer to thicken downstream more rapidly than it would by vertical conduction alone. The ratio of the diameter of low viscosity plume heads to the diameter of thermals scales approximately as $(\lambda_h^*/\lambda_h^*)^{1/3}$, consistent with Rayleigh-Taylor theory. $Ra = 1 \times 10^8$, $Pe \approx 28000$, and $\lambda_t \approx 10^3$. 
Figure 9.3: Shadowgraph images of transient 2: The evolution from steady-state active-lid convection following cessation of the imposed large-scale flow.  

a) Steady-state active-lid convection. Dark bubbles show the geometry of the imposed motions (white arrow). Rising low viscosity plumes are drawn into the large-scale flow. Plume conduits are clustered near the left side of the tank. 

b), c) The belt is turned off and plumes rise more vertically. Heads and trailing conduits are evident in c). $Ra = 1 \times 10^7$ (during steady-state active lid), $Pe \approx 26000$, $\lambda_t \approx 10^3$, $\lambda_h \approx 16$. 


9.2 Quantitative results

9.2.1 Transient 1

To characterize the evolution in flow regime as a function of $Pe$ through transient 1 we analyze local time series of temperature, $\theta^*$, heat flux, $q^*$, and the viscosity ratio across the hot thermal boundary layer, $\lambda_{th}^*$, acquired from both stack 1 and stack 2 (Figure 8.1). It is important to note that whereas the stacks capture the hottest temperature in the thermal boundary layer (the hot boundary temperature), by virtue of their design they do not necessarily capture the lowest temperature carried by cold material that advances across the hot boundary. Consequently, our absolute measurements at these locations likely underestimate the effects of the spreading cold front on the local temperature and viscosity variations. However, relative differences between experiments (and between each experiment and the stagnant lid case) are preserved such that we may characterize and compare flows in a self-consistent way.

9.2.2 Temporal dynamics: Frequency of thermal formation

Figures 9.4a and 9.4b show time series for the internal temperature for stagnant lid convection under steady-state conditions along with the corresponding power spectra. Two observations are noteworthy. First, as mentioned above, the mean interior temperature, $\theta \simeq 0.76$ and convection is in the form of intermittent thermals expressed as positive temperature anomalies, consistent with previous work (Jellinek & Manga, 2004). Second, we identify distinct frequencies for the formation of hot and cold thermals in both the hot and cold thermal boundary layers, the ratio of which is consistent with that found by Schaeffer & Manga (2001).

As outlined above, the spreading of cold fluid along the hot boundary influences the temporal (and spatial) dynamics of the hot boundary layer. To analyze these transient data in the spectral domain we low pass filter the data and remove the secular trend such that the time series are quasi-stationary. Because frequency resolution is ultimately limited by the number of convective instabilities that can occur during length of the
Figure 9.4: Plots showing the temporal dynamics of the hot thermal boundary layer during stagnant-lid convection and transient 1. 

a) Time series of internal temperature for run 15 (Table 8.2); b) power spectra for the same experiment based on time series of temperature recorded in both the hot TBL (stack 2) and cold TBL during stagnant-lid convection. Frequencies for the formation of hot and cold thermals are found in both boundary layers, indicating that convective instabilities in the hot and cold boundary layers are influenced by sinking (cold) and rising (hot) thermals, respectively (Moresi & Solomatov, 1995). c) Power spectra from a time series of temperature from stack 2 obtained during transient 1. The advection of cold material along the hot boundary causes the frequency of hot thermal formation to increase.
transient it is enhanced for low-$Pe$ flows. Nevertheless, comparison of Figures 9.4b and 9.4c illustrates how the power spectra at stack 1 evolve in response to the progressive stirring of cold boundary layer material during transient 1 for a run in which $Pe = 23000$. Comparison of the average hot frequency through the transient with that during the stagnant lid suggests that there is a shift to a higher frequency, consistent with the advective thickening of the hot thermal boundary layer discussed above (Figure 9.2).

### 9.2.3 Temperature and viscosity variations

The coexistence of thermals and plumes during transient 1 implies that lateral temperature, and thus viscosity, variations govern the structure of the flow in this regime. Figure 9.5 shows the evolution of local temperature variations recorded at stack 1 and stack 2 as a function of $Pe$ for four experiments. Each experiment begins in the stagnant lid regime. The belt is then turned on for $> 1$ full overturns. Only the experiments in Figure 9.5b, 9.5c and 9.5d reach steady-state active-lid conditions before the belt is turned off (or the conveyor belt system fails). The internal temperatures under these conditions are $0.60 < \theta < 0.66$. The interior temperature is greater than 0.5 because the measurements are local values and do not include lateral temperature variations arising due to the cavity-flow structure of the forced large-scale stirring.

Comparison of the data from both stacks characterizes the downstream thermal evolution of the advancing cold material and its influence on the structure of the vertical and lateral temperature variations within the thermal boundary layer. Following the onset of stirring the average and maximum cold temperatures decline from the stagnant lid values as the temperature drop from the hot boundary increases. Both the cooling of the thermal boundary layer and the vertical temperature gradients across each stack are maximized for the largest $Pe$ (Figure 9.5a). In addition, the local internal temperature is lower at stack 2 than at stack 1 because the cold front warms as it spreads across the hot boundary. For more moderate $Pe$ (Figure 9.5b,c) the internal temperature declines to a minimum value, where it remains. For the lowest $Pe$ experiment (Figure 9.5d) there is little difference to the stagnant lid case.

Figure 9.6 shows the local variations in $\lambda^*_h$ that correspond to the temperature varia-
Figure 9.5: Local temperature variations in the hot TBL at stack 2 (solid lines) and stack 1 (dashed lines) for different $Pe$ (runs 15, 14, 17 and 18 in Table 8.2), normalized to the average $\theta_s$ during steady-state stagnant-lid convection. The vertical lines mark the time when the belt is turned on (long dashes) and turned off (short dashes). $\Delta T$ across the hot thermal boundary layer was measured 4 cm above the hot boundary in stack 1 and stack 2. Since the position of these thermocouples was fixed, they may not have captured the full extent of the temperature difference across the hot TBL.
Figure 9.6: Plot of local viscosity ratios measured at stack 2, normalized to the average $\theta_s$ during stagnant-lid convection for different $Pe$. Plot parameters are the same as in Fig. 9.5.
tions in Figure 9.5. As for temperatures, viscosity ratio increases when the belt is turned on, and is maximized for large $Pe$. Whereas for $Pe = 23000$, a nearly 6-fold increase in $\lambda^*_h$ is observed, little variation compared with the stagnant lid case is recorded for $Pe \sim 2300$. We note that the 6-fold increase in $\lambda^*_h$ is around a factor of 1.5 smaller than that which would be obtained from comparison of the ratio of plume to thermal head sizes and the discrepancy is due to the way in which stack 2 samples the vertical temperature field.

### 9.2.4 Local Heat Flux

Figure 9.7 shows local heat flux measured beneath stack 2 as a function of $Pe$ for five experiments. At the start of the transient $q^*$ increases linearly from 1 to a maximum, the magnitude of which increases with $Pe$. Subsequently, $q^*$ declines from this maximum and in some cases recovers a constant and lower value characteristic of steady-state active lid convection. Following cessation of the forced stirring $q^*$ decreases from the maximum to a steady-state stagnant lid value at a rate approximately proportional to $t^{1/2}$, consistent with a response determined by the time scale for thermal diffusion.

### 9.3 Comparison to Numerical Experiments

In Robin et al. (2007), my coauthors present a small suite of numerical experiments using the finite element code CITCOM, aimed at reproducing our qualitative results under conditions not available in the laboratory (see Robin et al. (2007) for details). In particular, they investigated the effect of a larger aspect ratio, a free-slip bottom boundary condition, and the inclusion of internal heating. They were able to reproduce $\lambda_h = 4$ in the case of stagnant lid convection, identical to our analogue modeling results. They then imposed the collapse of the stagnant lid by forcing circulation with a velocity boundary condition at the surface.

The resulting transient regime reproduced a mixed-mode of convection characterized by plumes coexisting with thermals in the exact manner observed in the laboratory, under both the no-slip and free-slip basal boundary conditions (Figure 9.8). Some difference
Figure 9.7: Time series of local heat flux for all of the experiments in Table 8.2. The onset and cessation of the forced flow is indicated with dashed lines as before.
Figure 9.8: Snapshots from several series of calculations of transient 1 (following the stagnant-lid regime) in the presence of a) free slip and b) no-slip basal boundaries. $Ra = 10^8$. Sidewall boundary conditions are symmetric, and the non-dimensional values of the surface velocities are +600 to the left of center, and -600 to the right of center. Approximately isoviscous thermals form in the hot boundary layer ahead of the advancing cold front, whereas low viscosity plumes, carrying a larger excess temperature, form behind.
was noted in that the viscosity ratio of the plumes to the surrounding mantle was less in the free-slip case due to the lack of squeeze layer (in this case, the thermal boundary layer under the cold downwelling grew by thermal conduction from the base alone). The inclusion of internal heating also reduced the power of the plumes and thermals, but the mixed-mode was observed nevertheless, for internal heating up to 97%. Internal heating reduced the buoyancy of the thermals and the plumes alike, hence a smaller fraction of the thermals reached the top of the mantle. We note, however, that in a 3D spherical earth, internal heating would have a reduced influence on the thermal profile of the mantle; hence, a cartesian model with little or no internal heating may be a more appropriate approximation (J. Lowman, personal communication).

Finally, the use of symmetric side boundaries in the numerical work meant that less heat was lost to the boundaries. In the laboratory experiments, viscous coupling to the side walls probably meant much of the coldest parts of the stagnant lid did not reach the lower boundary layer. Thus, the numerical runs achieved a $\lambda_h = 10^3$ in the active lid regime, roughly 10 times larger than the laboratory results were able to achieve. This implies that our laboratory underestimated the relative buoyancy of the highland-forming plumes to that of the coronae-forming thermals.

9.4 Conclusion

Following the initiation of subduction, the spatial and temporal dynamics of the hot thermal boundary layer depend on local conditions that vary in time. Results from our experiments and numerical simulations show that spreading of the cold stagnant lid along the hot boundary leads to a mixed mode of convection with approximately isoviscous thermals forming ahead of the cold front and low viscosity plumes forming behind. This regime will persist for the time required for the cold material to cover the hot boundary. For a given system aspect ratio the longevity of the mixed mode regime decreases with increasing $Pe$ because the time scale to cover the hot boundary with cold material is reduced. The magnitude of the local temperature and viscosity variations giving rise to low viscosity plumes increase with $Pe$. These variations correspond also
with variations in heat flux. One interesting result is that the local heat flux can exceed the steady-state active-lid value during transient 1.

Comparison with our numerical simulations suggests that this regime will also emerge in the presence of intermediate extents of internal heating, and for no- and free-slip basal boundaries. However, the relative timing and spatial relationship between thermals and low viscosity plumes probably depends quantitatively on the mechanical coupling to the hot boundary and may depend on the relative proportions of internal to basal heating. In particular, thermal formation observed directly ahead of the advancing cold front (Figure 9.2) may be enhanced even further by the lateral advection, or ‘bulldozing’, of boundary layer fluid if the basal boundary condition is free-slip. In addition, the time scale for plume-forming instabilities upstream from the cold front may be reduced if a significant squeeze layer is trapped during spreading, a feature which is enhanced for rigid boundaries. The spacing of plumes and thermals will depend on both the mechanical coupling to the hot boundary and on variations in the vertical and lateral viscosity structure of the hot thermal boundary layer (e.g. Lister & Kerr (1998)).

A full analysis of the evolution of such a bimodal, transient hot TBL on a spherical planet, where the relative surface areas of the lithosphere and core-mantle boundary is greater, are beyond the scope of this paper. Indeed, the distribution of cold downwelling material on the CMB and the resulting temperature gradients at the CMB may be considerably different than those presented in our simple laboratory models. Details of the geometry of lithospheric break-up and the role of phase-changes in the mantle will also influence the final distribution of thermals and plumes as they impinge on the newly formed lithosphere. Nevertheless, our models support the concept of the coexistence of thermals and long-lived plumes during a transient phase of mantle convection, as envisioned by Johnson & Richards (2003).
Chapter 10

Summary and Discussion

10.1 Summary

Our experimental results combined with the numerical results presented in Robin et al. (2007) show that the contemporaneous coexistence of uncompensated BAT coronae and the Atla and Beta highland regions may indeed be explained as a result of a mixed-mode style of mantle convection from the core-mantle boundary (i.e. Figure 7.1b). Such a regime can arise during a thermal transient following a large-scale lithospheric overturn. It is expected to persist for a time scale that depends on the spatial extent and geometry of the overturn, as well as the rates and styles of subduction and subsequent mantle stirring. That this regime is observed for no- and free-slip basal boundary conditions suggests also that it will emerge if Venus has a liquid or a solid core (Nimmo, 2002; Konopliv & Yoder, 1996). Significantly, this style of upwelling flow is not consistent with our and previous laboratory experiments and numerical studies on stagnant-lid and active-lid convection under thermally steady-state conditions. Thus, whereas we confirm the plausibility of the model proposed by Johnson and Richards (Johnson & Richards, 2003) (Figure 7.1), we also identify the highly restrictive conditions in which such a regime may occur.
10.2 The coexistence and relative timing of Atla and Beta Regio and BAT coronae

A constraint on the relative timing of uncompensated BAT coronae and the Atla and Beta highlands may be drawn from our work. Johnson & Richards (2003) suggest on thermal grounds that the population of BAT coronae due to mantle thermals are younger than the isostatically compensated coronae distributed broadly over the surface of Venus. That is, assuming all coronae are initially a surface expression of mantle thermals, one way to distinguish the two populations of coronae is to explain the current positive gravity anomalies associated with BAT corona in terms of thermal buoyancy sources in the mantle that decay over time. Thus, the compensated coronae have equilibrated thermally by thermal diffusion and perhaps melt production (Dombard et al., 2002).

A second characteristic that defines the two populations is the geometric concentration of uncompensated coronae within the BAT region. Johnson & Richards (2003) suggest that the focussing of these features within BAT is due to a combination of effects related to the spreading of cold sublithospheric drips at the core-mantle boundary and upwelling flows into Atla and Beta (Figure 7.1b). Alternatively, as investigated here, the clustering of thermals as well as the formation of low viscosity axisymmetric upwellings giving rise to Atla and Beta, may be governed by the spreading of an overturned layer of cold lithosphere at the core-mantle boundary: clustered thermals form ahead of the advancing front of cold lithosphere as it ‘bulldozes’ and thickens the hot TBL ahead of it, and low-viscosity plumes form behind (Figure 9.2). Indeed, the concentration of dynamically supported coronae within BAT is not inconsistent with thermals being focused by an axisymmetric mantle return flow occurring in response to a lithospheric overturn in a spherical geometry (Zhong et al., 2000). The relative timing of the surface expressions of both upwelling features then depends on the time scales for their formation and rise through the Venusian mantle.

Quantitative constraints on the timescales for the formation of both types of upwelling features at the hot boundary are complicated by interactions between the spreading cold fluid, the hot thermal boundary layer and the hot boundary itself. Figures 9.2 and
9.4 suggest that thermal formation is enhanced directly ahead of the advancing front due to advective thickening of the thermal boundary layer. Consequently the period of thermal formation is less than that which would occur downstream of the cold front by thermal diffusion alone. However, the magnitude of the effect depends on $Pe$, which is not constrained for Venus, and on the mechanical coupling to the core-mantle boundary. The time scale of plume formation depends on the initial thickness of the trapped squeeze layer (no-slip boundaries) as well as the rates of vertical thermal diffusion and lateral advection (no- and free-slip boundaries).

Whereas constraints on the timescale of formation are not straightforward, estimates of the relative times for plumes and thermals to rise across the mantle can be obtained readily. Such estimates thus indicate a lower bound on the relative ages of uncompensated BAT coronae and the Atla and Beta regions. We note that both thermals and plumes are observed to form closely in time in all experiments and simulations. We assume that mantle deformation is in the diffusion creep limit and take the viscosity $\mu = \mu_0 \exp(-\gamma T)$, where $\mu_0$ is a reference viscosity and $\gamma$ is the rheological temperature scale. Low viscosity plume heads are expected to rise faster than thermals because they are both larger and carry a greater excess temperature. The ratio of the time scale of a thermal to ascend across the mantle to that for a nascent plume head (i.e. starting plume) is $\tau_{th}/\tau_{pl} \sim (\Delta T_{pl}/\Delta T_{th})(d_{pl}/d_{th})^2 \sim (\Delta T_{pl}/\Delta T_{th})(\lambda^{pl}_{h}/\lambda^{th}_{h})^{2/3}$, where $d_{pl}$ and $d_{th}$ are expected to scale with the respective critical thermal boundary layer thickness such that $d_{pl}/d_{th} \sim (\lambda^{pl}_{h}/\lambda^{th}_{h})^{1/3}$ (e.g. Lister & Kerr (1998)). We take $\gamma = 0.0145$, which gives $\lambda^{th}_{h} \approx 4$ (the stagnant lid value) for a thermal excess temperature $\Delta T_{th} \approx 100^\circ C$ as well as $\lambda^{pl}_{h} \approx 100$ and $\lambda^{pl}_{h} \approx 200$ for plume excess temperatures of $\Delta T_{pl} \approx 200^\circ C$ and $\Delta T_{pl} \approx 300^\circ C$, consistent with parameters inferred for low viscosity mantle plumes in the Earth (e.g. Jellinek & Manga (2004)). Assuming that the mean diameter of isostatically compensated coronae indicate the average diameter of underlying mantle thermals we take $d_{th} \approx 200$ km. Applying these values we obtain $d_{pl}/d_{th} \approx 1.6 - 2.7$ and $\tau_{pl}/\tau_{th} \approx 5 - 20$. In addition, for $200 \leq \Delta T_{pl} \leq 300^\circ C$, an average Venusian mantle viscosity of $5 \times 10^{20}$ Pa-s and reasonable physical properties (Nimmo & McKenzie, 1996; Solomatov & L.-N. Moresi, 1996; Nimmo & McKenzie, 1998) the time scale for a low
viscosity plume to rise across the full depth of the mantle is expected to be 60 - 20 Myr, respectively (Lamb, 1945; Griffiths, 1986). In contrast, nearly isoviscous thermals are expected to take around 300 Myr to traverse the Venusian mantle.

If the plumes and thermals forming in response to a lithospheric overturn emerge from the core-mantle boundary region closely in time, it is reasonable to expect the Atla and Beta highland regions to precede BAT coronae by > 250 Myr. With additional information about the uplift history of the Atla and Beta highlands, this relative timing also constrains the absolute age of BAT coronae. Vezolainen et al. (2003) apply a combination of results from geological, geomorphological and cratering studies to argue that the time scale for the uplift of Beta Regio is less than about one-half the mean surface age. Assuming a mean surface age of 700-800 Myr, this result implies that the uplift of Beta occurred over the last 350-400 Myr, which is comparable to the time scale for a thermal to rise across the mantle. Thus, it is reasonable to suggest that some fraction of the uncompensated BAT coronae may have formed within the last 100 Myr.

Based on the preceding discussion, we propose the following rough timeline of events: i) Venus experiences a gravitational collapse of the stagnant-lid (700 Ma); ii) pieces of the cold lid reach and spread across the CMB, forming squeeze layers beneath them and ‘bulldozing’ the hot TBL ahead of them (500 Ma); iii) low viscosity plumes from the squeeze layer reach the surface and form Atla and Beta Regio (350 Ma); and iv) thermals formed in the bulldozed TBL between the advancing cold fronts responsible for the Atla and Beta plumes finally reach the surface, concentrated in the BAT region (< 100 Ma).

### 10.3 Future Work

As explained in the General Introduction to this thesis, this project was cut short by the dismantling of our laboratory. However, our results suggest a number of directions for future study, some of which would have been tackled if the project had continued.

Analyses of the spatial and temporal relationships between thermals and low viscosity plumes for a range of $Pe - Ra - \lambda_t$ conditions in Cartesian and spherical systems would be useful for understanding the geometric distribution and timing of resulting coronae and
plume-related highlands. Indeed, the geometric relationship between the BAT coronae and the BAT highlands themselves may provide constraints on the scale and geometry of a lithospheric overturn on Venus. An additional interesting result is that during a transient following an overturn the local core heat flux can exceed the steady-state active-lid value. Depending on the spatial distribution and magnitude of such heat flux maxima, such a condition raises the possibility of a short-lived core dynamo.

Future numerical work of the transient following the collapse of a stagnant lid could include a greater variety of internal to basal heating ratios, initiating transient regimes by failure of the viscoplastic rheology instead of by an imposed upper boundary velocity condition (which would allow for variable convective cell sizes), using more realistic non-Newtonian rheologies, and including a phase transition at 740 km.

Another interesting line of research would be to analyze the response of the Venusian crust to impinging thermals, to see whether the range of coronae morphologies can be reproduced. Several mechanisms for coronae formation and evolution have been proposed; however, none of them account for the full range of coronae sizes and morphologies. Moreover, these models make no attempt to account for the petrological data returned by the Venus landers. Most corona models are of a rising axisymmetric density anomaly that flattens into a disk as it meets a strong upper layer (Musser & Squyres, 1997). Surface deformation begins as a dome accompanied by extensional radial faulting, followed by a plateau. This simple model accounts for the broad plateaus associated with some coronae, but not for most coronae morphologies (rims, depressions and moats). Musser & Squyres (1997) suggest the moat may be due to visco-elastic relaxation of the surface under a load; however, they do not model this deformation explicitly, and it appears to be inconsistent with most moat dimensions. (Koch & Manga, 1996) perform a more rigorous analysis of the surface deformation due to a diapir spreading at a level of neutral buoyancy, which could be within the lithosphere, between the mantle and the crust, or at the gabbro-eclogite phase transition. This ‘spreading-drop’ model is more successful at reproducing rimmed depressions at a late stage of coronae formation, but not moats. They suggest that moats may be related to ‘thermal effects such as cooling of the nose of the spreading diapir’, but do not model it explicitly. Smrekar & Stofan (1997b) and
Sandwell & Schubert (1992) have advanced models calling on lithospheric delamination and subduction at coronae edges, but these only work for the largest coronae. It would be of interest to test the visco-elastic response of a buoyant thermal at a number of levels in the crust and lithosphere, including the effect of lithospheric or crustal melting in response to a localized and transient heat source (e.g. Dombard (2006)).

Finally, it would be deeply satisfying to reproduce our laboratory experiments with an improved apparatus. Our apparatus failed on a number of occasions, and needed to be completely rebuilt on one occasion, which is why most of our usable results were not achieved until after the completion of my M.Sc. This was largely due to the highly viscous and sticky nature of cold corn syrup, which made the operation of our mobile belt extremely difficult. Even successful attempts at initiation subduction could not be sustained for long periods, and several motors were burnt out in the process. Moreover, the gap between the cold heat exchanger and the belt meant that the stagnant lid was not as cold as it could have been. If this experiment were to be repeated, I would primarily: i) build a tank with a higher aspect ratio to minimize the viscous coupling of the cold downwelling to the sides of the tank; and ii) have the mobile belt act as the cold heat exchanger as well, with cold water circulating directly through the belt. This would minimize the stress on the rotating motor, and increase the thermal contact between the syrup and the cooling source.
Part III

The thermal effect of fluid flows in AECL’s Tunnel Sealing Experiment
Plutonic (crystalline) rocks in stable tectonic areas are under consideration for permanent disposal of high-level nuclear waste (mainly heat-generating waste fuel from nuclear reactors) in North America, Europe and Asia. In Canada, this model is being tested for a variety of different configurations at a depth of 400-1000 m in granitic plutons of the Canadian Shield. Used fuel in resistant containers would be buried in emplacement rooms in vertical or horizontal boreholes, which would then be backfilled with a mixture of clay-based buffers and backfills (typically mixtures of bentonite clay and sand) (Guo et al., 2005b). These chambers would also include bulkhead seals placed in strategic locations in tunnels and shafts and at the entrance to emplacement rooms. In addition to blocking flow directly out of tunnels, these seals would act to minimize fluid flow out of the chambers through the rock by way of excavation damage zones (EDZs). Thus, the flow of water and contaminating radionuclides should be contained by a system of engineered barrier systems and natural rock.

Two materials considered for the sealing bulkheads (concrete and clay) were tested with a full-scale in situ Tunnel Sealing Experiment (TSX). ‘At the time of its construction and operation the TSX represented the first installation of full scale, keyed tunnel seal in crystalline rock that was specifically designed to examine the effectiveness of keying a tunnel to prevent seepage past bentonite or concrete materials. The TSX was not a test of a specific design of seal but rather to evaluate the individual performance of two sealing materials (bentonite and concrete) that would likely be used together in the
construction of an actual repository seal’ (Dixon et al., 2007).

During the experiment, however, it was noted that the temperatures measured in the bulkhead were up to $20^\circ C$ colder than what had been predicted by thermo-hydro-mechanical models. Dismantling the experiment did not reveal a reason for this discrepancy, which remains unexplained. It does not appear to be a problem with the modeling procedure. In this chapter, we explore three possible physical reasons for the unexpected heat transfer properties of the system, using the finite element software Comsol Multiphysics 3.5a. The work presented here will focus on the clay bulkhead, although the main conclusions affect both bulkheads equally.

Figure 11.1: Configuration of the tunnel sealing experiment. From Dixon et al. (2007)

The TSX was carried out at the 420 m level of the Underground Research Laboratory (URL) of Atomic Energy of Canada Limited (AECL) in Whiteshell, Manitoba, in collaboration with the Japanese Nuclear Cycle Development Institute (JNC), Agence nationale pour la gestion des déchets radioactif (ANDRA), France, and the Waste Isolation Pilot Plant (WIPP), USA.
Figure 11.2: Details of the tunnel seal design. See Figure 11.1 for scale. From Martino et al. (2007)

11.1 TSX design and construction

TSX design is shown in Figure 11.1. Because of excavation-induced damage which extended to $\sim 0.5 \, m$ into the rock around the periphery of the tunnel (the EDZ), bulkheads were carefully keyed into the rock to limit axial flow from the tunnel through the rock (Martino et al., 2007).

One seal was composed of highly compacted sand-bentonite blocks, while the other was constructed with low-heat, high-performance concrete (LHHPC) (Figure 11.2). The chamber between them was filled with sand (Figure 11.1). These materials were emplaced from the clay bulkhead side to the concrete bulkhead side (Martino et al., 2007).

The clay bulkhead was built by emplacing pre-compacted blocks ($0.1 \, m \times 0.36 \, m \times 0.20 \, m$) by hand, using a layout aimed at limiting fluid flow through the contact between the blocks (Figure 11.2) (Martino et al., 2007). It was supported on the tunnel side by a steel restraint, and on the chamber side by a 30 cm thick backfill made of 90% sand and 10% clay (Guo et al., 2006). Sensors were fit between the clay blocks as they were placed. The walls of the clay seal were lined with pneumatically sprayed shot-clay liner 5 to 60 mm thick to minimize fluid flow to the surrounding rock (Martino et al., 2007).

The bottom half of the Sand Chamber was filled and then compacted with a vibratory plate compactor while the upper half was pneumatically emplaced but not compacted.
Figure 11.3: Thermistor locations on the vertical section through the axis of the TSX. See Figure reffig:DixonEtAl2007Fig3 for scale. Temperature in the concrete bulkhead was measured by VSM02T, VSM08T, VSM19T, VSM24T, VSM27T and TPC28T, temperature in the clay bulkhead by PSY47T, PZ5T and PZ6T, temperature for the inlet headers by PZ22T and PZ30T, temperature for the outlet headers by PZ28T and PZ20T, temperature in the rock by EXT2-2T, EXT2-3T, EXT2-4T, EXT2-5T and EXT2-6T and pore pressure in the rock by HGT1-1, HGT1-2, HGT1-3, HGT1-4 and HGT1-5. From Guo et al. (2005a) (Martino et al., 2007). The concrete bulkhead was poured in against a 25 cm thick cast concrete wall, and the sensors were cast within in (Martino et al., 2007).

The sand chamber was incrementally pressurized with water up to 4 MPa during Phase 1 of the TSX, followed by heating to $\sim 84^\circ C$ by circulating heated water in the sand-filled chamber during Phase 2 (Guo et al., 2005b) (Figure 11.4). The heating phase was divided into two parts: in Stage 1 (170 days), the temperature of the inlet heaters was raised to and maintained at $65^\circ C$; in Stage 2 (251 days), the temperature of the inlet heaters was raised to and maintained at $95^\circ C$ (Guo et al., 2006). Heating progressed by thermal convection of the heated and pressurized water in the permeable sand, and by
Figure 11.4: Layout of the TSX heating system. From Guo et al. (2005a)

conduction in the concrete and clay seals (e.g. Dixon et al. (2007); Guo et al. (2005b, 2006); Martino et al. (2007)). The TSX was monitored with a collection of thermistors and hydraulic head gauges (Dixon et al. (2007)), which were in use throughout both phases of the TSX (Figure 11.3).

The structure and test conditions were based on an extensive series of numerical models performed before and during the run of the TSX (e.g. Guo et al. (2005b)). Thermo-hydro-mechanical (THM) models of the TSX were largely performed using MOTIF (Model of Transport In Fractured/porous Media), developed by AECL and successfully used for international collaborations on similar projects. MOTIF is a three-dimensional finite element program which simulates fluid flow and heat transport in fractured/porous media, as well as solute transport (not discussed here) (e.g. Guo et al. (2005b); Guo & Dixon (2009)). Some calculations were performed in parallel with the finite element program FLAC (Fast Lagrangian Analysis of Continua), developed by Itasca (Guo et al., 2005b). After decommissioning, the TSX was closely scrutinized to understand differences between the numerical predictions and actual outcomes, as well as structural changes not recorded by the sensors.
11.2 Comparison of MOTIF models and observations at the TSX

A few discrepancies were noted between the predicted outcomes and measured results. For instance, the clay bulkhead/key was expected to be saturated throughout the entire bulkhead uniformly; instead, there was a preferential flow path between clay blocks, and in the unsaturated shotclay between the blocks and the surrounding rock in the initial stages of saturation (Guo & Dixon, 2009). Nevertheless, complete saturation was reached in the time estimated by the models. Moreover, as clay absorbed water during the saturation stage, it tightened the fit between clay blocks, reducing eventual seepage through the bulkhead.

Seepage through the clay bulkhead translated into an effective hydraulic conductivity of $8.6 \times 10^{-12}$ m/s (1 mL/min) versus $1 \times 10^{-10}$ m/s (10 mL/min) for the concrete bulkhead (which was reduced to 1 mL/min during the heating phase as the concrete thermally expanded) (Martino et al., 2007). Such low seepage rates had no effect on the transport of heat from the Sand Chamber to the bulkheads. In addition, it must be kept in mind that these seepage rates are for a limitless water supply and a 4 MPa hydraulic gradient, whereas during operation of the DGR the pressure gradient would be much lower and there would be very restricted water supply (Martino et al., 2007).

On decommissioning, a 3 cm gap was found at the crown of the sand-filled chamber, in the upper portion of the sand, which had not been compacted prior to operation (Martino et al., 2007). Part of it had been embayed by clay, suggesting that at least some of the gap existed during the experiment (Martino et al., 2007). Due to the expansion of the clay with water content, the clay-filled gap was not likely a locus for fluid flow. In addition, micro-seismic sensors in the rock suggest that most of the gap formed on decommissioning as the tunnel was depressurized and drained (Martino et al., 2007).

A major discrepancy was found between the predicted and observed temperatures of the clay and concrete seals during the second phase of the TSX (Martino et al., 2007; Guo & Dixon, 2009; Guo et al., 2005b). The observed temperatures as recorded by centrally located thermistors in both seals (Figure 11.3) were close to the expected temperatures
(a) Simulated and measured temperatures at three locations in the clay bulkhead

(b) Simulated and measured temperatures at three locations in the concrete bulkhead

Figure 11.5: From Guo et al. (2005b)
for the first 51 days, at which point the observed temperatures increasingly diverged from the predicted ones with time (Figure 11.5) (Guo et al., 2005b). The drop in temperature at 51 days ‘was attributed to a leak from a broken pipe in the circulation system that required several hours to fix and resulted in a loss of a large volume of heated water’ (Guo et al., 2005b). By the end of the experiment (day 420 of the heating phase), the temperature in the clay bulkhead had diverged from the expected temperatures by $\sim 20^\circ C$ (Figure 11.5).

In order to match the models with the measured temperatures, the thermal conductivity of the clay backfill was adjusted on back analysis from the original 1.6 $W/m/K$ to 0.26 $W/m/K$ at the end of the heating phase (Figure 11.5) (Guo et al., 2005b, 2006). There is no physical basis for adjusting the thermal conductivity of the backfill in this manner, but it was necessary to match the data. A similar adjustment on back analysis was performed for the concrete bulkhead (Figure 11.5), but will not be discussed further here. However, the temperatures measured in the surrounding rock fit the expected profile quite well. Hence, the thermal discrepancy is not thought to stem from a problem in the THM calculations, but from a physical process which was not accounted for by the models (Guo et al., 2005b).

![Conceptual model for the formation of air bubbles](image)

**Figure 11.6:** Conceptual model for the formation of air bubbles. From Guo et al. (2005b)

To our knowledge, the discrepancies in modeled and measured temperatures in both the concrete and clay bulkheads has not as yet been resolved. They have generally been attributed to ‘changing material properties as the clay bulkhead warms, local variations in clay properties causing channels of warmer material to form, or possibly data acqui-
sition issues or inadequacies in the model’ (Guo et al., 2005a), but no models have been published which test these ideas.

The following three possible scenarios have been suggested for the discrepancies in the clay bulkhead:

1. The formation of air bubbles coming out of solution as the water (which had not been de-aired) was heated (Guo et al., 2005b; Guo & Dixon, 2009). The suggestion is that small gaps may have created insulating air layers in key locations near the bulkheads or the temperature sampling points (Figure 11.6). These were not found on decommissioning, but may have been too small to be noticed or have been collapsed by the decommissioning process.

2. The formation of water-filled pockets in the clay. This suggestion was based on the fact that 1 – 10 cm air pockets were discovered in the low-density clay (near the clay-wall contact) on the upstream side of the clay bulkhead in a region that had been water saturated (Guo et al., 2006). Guo et al. (2006) suggest that voids of unknown geometry may have formed throughout the clay bulkhead due to swelling, sand slumping and measured small displacements in the clay bulkhead and backfill (Martino et al., 2007) which would all contribute to an change in the effective thermal conductivity of the clay seal.

3. The formation of micro-channels in the sand chamber (Guo et al., 2006). Thermal stresses induced in the clay backfill by the sudden drop in temperature at day 51 could have resulted in structural changes which could allow significant amounts of fluid flow not accounted for in the modeling. Resulting micro-channels in the otherwise homogeneously permeable sand would have limited heat transport to the bulkheads to conduction alone in some areas. Since the MOTIF models modeled heat transport in the sand chamber as both conduction and convection, such a change in effective thermal conductivity would not have been taken into account by the models (Guo et al. (2006)).

Here we will present models of the clay bulkhead half of the TSX testing the three hypotheses put forth by the TSX modeling team, using the commercially available finite
element software Comsol Multiphysics (versions 3.4 and 3.5a). All our models aim to reproduce the temperatures measured in the final days of the experiment (day 420 - see Figure 11.5a), which are assumed to be steady-state, without adjusting the measured thermal properties of the materials involved.
Chapter 12

Numerical Experiments

12.1 The finite element code

Comsol Multiphysics (CM) (formerly FEMLAB) is a finite element solver software for problems in physics and engineering. It offers a wide variety of applications or ‘Modules’, ranging from Chemical Engineering to AC/DC, and is particularly adaptable to coupling different systems of equations across different modules (‘multiphysics’). It is also possible to set up tailored systems of coupled partial differential equations, and to run CM with an interface to Matlab.

The thermo-mechanical models presented here couple equations from the general Multiphysics package (the Fluid Dynamics module, which solves the incompressible Navier-Stokes equation, and the Heat Transfer module, which solves the heat equation, with or without convection) and the Earth Science module (which solves the same equations, but with the inclusion of multiphase flow in porous media (the Brinkman equations)).

12.1.1 Fluid dynamics equations

The Navier-Stokes (N-S) application mode solves the momentum balance equation

\[
\rho \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot [\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \mathbf{F}
\]

(12.1)
and the equation of continuity for incompressible fluids

\[ \nabla \cdot \mathbf{u} = 0 \quad (12.2) \]

where \( \mathbf{u} \) is the velocity field, \( \eta \) is dynamic viscosity, \( \rho \) is density, \( p \) is pressure, and \( F \) is a volume force. In all our models, \( F \) is gravity, given as \( F_y = -\rho(T)g \), where \( T \) is temperature.

The Earth Science module offers the Navier-Stokes equation with the inclusion of flow through porous media, known as the Brinkman equations. They are described as an extension of Darcy’s law to include the dissipation of kinetic energy by viscous shear.

Darcy’s law describes the flux per unit area of viscous fluid through an aperture under an applied pressure gradient, and is defined as

\[ J = -\frac{\kappa}{\eta} \nabla P \quad (12.3) \]

where \( J \) is the flux (in \( m/s \)) and \( \kappa \) is the permeability (in \( m^2 \)), and \( P \) is pressure (in \( Pa \)).

The Brinkman equations can be thought of a combination of Navier-Stokes flow through large apertures or pores, and Darcy’s law for flow through permeable regions with small pores. This is applied using an effective viscosity which includes the frictional force between the fluid and the pores, which allow Darcy’s law to be applied to the boundary between Navier-Stokes type fluid flow and flow through permeable media. The Brinkman equations are solved by Comsol in the form

\[
\frac{\rho}{\varepsilon_p} \frac{\partial \mathbf{u}}{\partial t} + \frac{\eta}{\kappa} \mathbf{u} = \nabla \cdot [p \mathbf{I} + \frac{1}{\varepsilon_p} \{ \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2\eta}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \}] + F \quad (12.4)
\]

\[ \rho \nabla \cdot \mathbf{u} = 0 \quad (12.5) \]

where \( \varepsilon_p \) is porosity, and the other variables are as defined above.

Once all the physical parameters for a particular media are defined (some of which are available from Comsol’s Materials Library), it is straightforward to set the boundary conditions for each edge as drawn in the geometry. In all our models, we applied the no-slip \( (\mathbf{u} = 0) \) boundary conditions for most exterior boundaries, except for the case where we modeled flow of heated water through the sand chamber. In that domain we set a normal inflow velocity into the sand chamber and an outflow velocity out of it at locations corresponding to the inlet and outlet as shown in Figures 11.3 and 11.4.
12.1.2 The heat equation

The basic equation describing heat transport is

\[ \rho C_{eq} \frac{\partial T}{\partial t} + \nabla \cdot (-k_{eq} \nabla T) = Q - \rho C_L u \cdot \nabla T \]  \hspace{1cm} (12.6)

where \( C_{eq} \) is effective volumetric heat capacity, \( T \) is temperature, \( k_{eq} \) is the effective thermal conductivity, \( u \) is the velocity field (input from the coupled N-S equations), \( C_L \) is the volumetric heat capacity of the moving fluid and \( Q \) is a source term. Most of our modeling domain is purely conductive, in which case \( u = 0 \) and \( k_{eq} \) and \( C_{eq} \) are the conductivity and heat capacity of the solid. Models which couple the N-S equations to the heat equation use the conductivity and heat capacity of the moving fluid. In the domains where we couple the Brinkman equations with the heat equation, \( k_{eq} \) is defined by a power law \( k_{eq} = k_L^\theta k_P^{(1-\theta)} \) where \( k_L \) is the conductivity of the liquid, \( k_P \) is the thermal conductivity of the solid matrix, and \( \theta \) is the volume fraction of the liquid. Similarly, \( C_{eq} \) is a volume average of the heat capacities of the two components.

As with the N-S equations, boundary conditions are imposed at the push of a button for each boundary. In our models, we typically use temperature and thermal insulation for external boundaries together with temperature and continuity conditions for internal boundaries.

12.1.3 Solving the equations

The N-S equations are notoriously difficult to converge, even in cases where the flow should be laminar and time-independent. Rather than making our models time-dependent, we used CM’s built in parametric solver. This permits one to gradually approach a parameter value by using the previous solution as the starting point for the next. These values are defined as solver parameters. For instance, one can gradually increase the driving force by ramping up the non-physical parameter ‘\textbf{damp}’ in \( F = F_y = -\textbf{damp} \rho(T)g \), or decreasing the viscosity \( \eta \), or decreasing the permeability in the Brinkman equations. Other tricks to stabilize the N-S/Brinkman equations include artificially fixing a pressure point in the domain, taking increasingly small steps in the parametric solver, and
using artificial stabilization techniques such as isotropic diffusion, streamline diffusion and crosswind diffusion (see the Comsol Multiphysics Modeling Guide for details). No attempt was made to use a time-dependent or transient solver, as any physically realistic solution for the TSX should be steady-state (i.e. should not involve large volumes of freely flowing turbulent fluid).

Another key factor was building the mesh. Small mesh sizes quickly become too expensive; any calculation with more than 12000 or so degrees of freedom did not run. However, Comsol allows one to define tight meshes on boundaries, in boundary layers, or in selected subdomains, while keeping the conductive portions of the model very coarsely meshed. We can also change the relative tolerance of the solver from the default of $10^{-6}$, which on visual inspection appeared to give reasonable results. Nevertheless, for some geometries the solution for the N-S equation did not converge for realistic viscosities ($\eta \approx 10^{-3} \text{ Pa s}$ for water). The Brinkman equations were considerably more stable except for very high permeabilities, since the effective viscosity is reduced due to friction with the pores.

### 12.2 Model Geometry

The model set up was based on the TSX geometry as shown in Figures 11.4 to 11.3 and in Guo et al. (2006). For computational reasons, we modeled only half the TSX in most models involving fluid flow, including only the Clay Bulkhead (see Figure 12.1). Since the boundary dividing the model and the un-computed other half was reflective or symmetric, the results are applicable to the concrete bulkhead side as well, except in the case of flow in the bulkhead itself.

Physical parameters were mostly taken from Guo et al. (2005a) and Guo et al. (2006) (see Figure 12.2). Since there were inconsistencies in the published thermal conductivities, we specify which was used in each case presented below. For all models involving fluid flow, the fluid is water, and its properties are the default ones in the Comsol Materials Library; these are all standard and temperature-dependent where applicable. It should also be noted that the densities reported in Guo et al. (2005a) and Guo et al.
Figure 12.1: Model Set Up. This figures shows the geometry used in most of our calculations. We model only half the TSX, including the clay bulkhead only. Thermal boundary conditions (BCs) are: dashed lines: temperature fixed at 14.35°C, the ambient rock temperature, which was also the air temperature behind the clay bulkhead; solid line (hot water inlet): temperature fixed at 85°C; dotted lines: continuity; dash-dot lines: thermal insulation (i.e. reflective boundary). Thermal conductivities ($k$) are marked for each material. Crosses mark the locations of thermistors. For models which included fluid flow, the outer boundaries of the domain were no-slip, and all internal boundaries were continuous.
Table III. Parameters of materials in the MOTIF model.

<table>
<thead>
<tr>
<th></th>
<th>Permeability (m$^2$)</th>
<th>Porosity</th>
<th>Dry density (kg/m$^3$)</th>
<th>Specific heat$^*$ (J/(kg·C))</th>
<th>Thermal conductivity (W/(m·C))</th>
<th>Longitudinal dispersivity (m)</th>
<th>Transverse dispersivity (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber sand</td>
<td>$6.25 \times 10^{-12}$</td>
<td>0.287</td>
<td>1850</td>
<td>820</td>
<td>1.0</td>
<td>0.37</td>
<td>0.037</td>
</tr>
<tr>
<td>Sand behind bulkhead</td>
<td>$6.25 \times 10^{-12}$</td>
<td>0.24</td>
<td>2000</td>
<td>820</td>
<td>0.5</td>
<td>0.06</td>
<td>0.006</td>
</tr>
<tr>
<td>Clay bulkhead</td>
<td>$1.0 \times 10^{-19}$</td>
<td>0.315</td>
<td>1900</td>
<td>810</td>
<td>1.6</td>
<td>0.26</td>
<td>0.026</td>
</tr>
<tr>
<td>Clay backfill</td>
<td>$1.0 \times 10^{-17}$</td>
<td>0.315</td>
<td>1860</td>
<td>820</td>
<td>1.6, 1.0$^a$</td>
<td>0.03</td>
<td>0.003</td>
</tr>
<tr>
<td>Concrete bulkhead</td>
<td>$3.0 \times 10^{-21}$</td>
<td>0.10</td>
<td>2430</td>
<td>900</td>
<td>1.8</td>
<td>0.35</td>
<td>0.035</td>
</tr>
<tr>
<td>Concrete wall</td>
<td>$6.25 \times 10^{-12}$</td>
<td>0.10</td>
<td>2430</td>
<td>900</td>
<td>1.8, 1.0$^a$</td>
<td>0.015</td>
<td>0.0015</td>
</tr>
<tr>
<td>Rock</td>
<td>$1 \times 10^{-21}$</td>
<td>0.005</td>
<td>2650</td>
<td>1015</td>
<td>3.5</td>
<td>0.6</td>
<td>0.06</td>
</tr>
</tbody>
</table>

$^*$Parameters for the dry materials were used.

$^a$Parameters were adjusted based on the results from back-analysis.

(a) From Guo et al. (2005a)

Table 2. Thermal and Mechanical Properties of Components

<table>
<thead>
<tr>
<th></th>
<th>Bulkhead sand filler</th>
<th>Clay bulkhead</th>
<th>Backfill</th>
<th>Rock</th>
<th>Chamber sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability (m$^2$)</td>
<td>$6.25 \times 10^{-12}$</td>
<td>$3 \times 10^{-19}$</td>
<td>$6.25 \times 10^{-17}$</td>
<td>$2 \times 10^{-23a}$</td>
<td>$6.25 \times 10^{-12}$</td>
</tr>
<tr>
<td>Thermal conductivity [W/(m·K)]</td>
<td>2.0</td>
<td>1.8</td>
<td>0.5$^a$; 0.36$^a$; 0.26$^a$</td>
<td>3.5</td>
<td>2</td>
</tr>
<tr>
<td>Specific heat [J/(kg·K)]</td>
<td>820</td>
<td>1,400</td>
<td>1,400</td>
<td>1,015</td>
<td>820</td>
</tr>
<tr>
<td>Young modulus (MPa)</td>
<td>600</td>
<td>200$^a$</td>
<td>200</td>
<td>5.759 × 10$^4$</td>
<td>100</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.3</td>
<td>0.315</td>
<td>0.315</td>
<td>0.207</td>
<td>0.3</td>
</tr>
<tr>
<td>Thermal expansivity (1/K)</td>
<td>$1.9 \times 10^{-5}$</td>
<td>$1.0 \times 10^{-5}$</td>
<td>$1.0 \times 10^{-5}$</td>
<td>$1 \times 10^{-6}$</td>
<td>0</td>
</tr>
<tr>
<td>Dry density (kg/m$^3$)</td>
<td>2,000</td>
<td>1,900</td>
<td>1,900</td>
<td>2,650</td>
<td>1,850</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.24</td>
<td>0.315</td>
<td>0.315</td>
<td>0.005</td>
<td>0.287</td>
</tr>
<tr>
<td>Biot’s coefficient</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.2</td>
<td>1.0</td>
</tr>
</tbody>
</table>

$^a$These values derived from back analysis.

(b) From Guo et al. (2006)

Figure 12.2: Material properties
(2006) are dry densities; however, for lack of any other data, these were the densities we used. Presumably these were also used in the MOTIF calculations.

Our results will be presented as colour plots of the temperature field with or without flow velocities represented by arrows, as well as temperature profiles as measured at locations approximating the locations of thermistors PZ20T, PSY47T, PZ5T and PZ6T in the TSX experiment (Figure 12.1).
Chapter 13

Results and Conclusion

13.1 Heat input: the Sand Chamber

The sand chamber was heated using a heated and pressurized flow of water (Figure 11.4). By modeling heat flow by convection through porous media, MOTIF models predicted the internal temperature of the sand chamber to be $\sim 84^\circ C$ throughout (Figure 13.1). Similarly, we reproduced these results using a fixed $\sim 85^\circ C$ temperature at the fluid inlet (Figure 13.2), and the permeabilities, porosities, and other physical properties given in Guo et al. (2005a) and Guo et al. (2006). The velocity of the fluid at the inlet and outlet was set at 0.003 $m/s$, a value which was comparable to the flow rate in the inlet pipe as given by Guo et al. (2005b), and which gave the best reproduction of the temperature distribution shown in Figure 13.1a. For some models (where we were not interested in fluid flow through the sand chamber) we used a fixed temperature source in the sand chamber to reproduce the temperature distribution of Figure 13.1a.

13.2 Conductive Cases

We reproduced the thermal profiles predicted by the original MOTIF models using measured thermal properties, and then changed the thermal conductivity $k$ to fit the measured data using the backfitted values from Figure 12.2. We term this the ‘conductive cases’ because, while the chamber is heated by the flow of hot water, the permeability
Figure 13.1: Thermal profiles of a) the sand chamber, assuming conductive and convective heat transfer from a hot water pumping system; and b) the concrete and clay bulkheads, assuming purely conductive heat transfer from boundaries of the sand chamber and using the best-fit thermal parameters based on back analysis (from Guo et al. (2005b)).
Figure 13.2: TSX temperature and velocity. The chamber is heated by hot water entering at the inlet and exiting at the outlet (see Figure 12.1). Thermal conductivity for the sand chamber is $2 \, W/m/K$; other values are the measured (not backfitted) properties listed in Guo et al. (2005a) and Guo et al. (2006). The resulting temperatures at our four sampling points (see Figure 12.1) were: PZ20T: $\sim 79^\circ C$; PSY47T: $\sim 69^\circ C$ ; PZ5T: $\sim 57^\circ C$; PZ6T: $\sim 46^\circ C$ (also see Figure 13.6).
in the chamber is quite low \( \kappa = 6.25 \times 10^{-12} m^2 \), and the rest of the model is heated by conduction alone.

### 13.2.1 Measured thermal parameters

Figure 13.2 show the results for a calculation using the measured thermal parameters of the clay backfill. Hereon in we will refer to this model as our ‘base case’. The 4 sampled temperatures compare well with those predicted by MOTIF for the same sampling points on day 420 of the experiment (Figure 11.5a). Our predicted values are \( \sim 2 - 3^\circ C \) lower than the predicted values plotted in Figure 11.5a, which is likely due to the use of different thermal conductivities (since it was not clear which were used for these MOTIF calculations), slightly different physical set-up of the model, or different mesh distribution and/or FEM interpolation schemes. However, these are small compared to the thermal effects we are attempting to account for.

We also tested the thermal profile for a 3D case (Figure 13.3), and compared the resulting temperatures with those of the 2D case. These models did not include fluid flow in the sand chamber, but used a fixed internal temperature of 84\(^\circ\)C instead. The calculated temperatures along the axis of the clay bulkhead was < 2\(^\circ\)C hotter in the 2D models than in the 3D models (Figure 13.4a). The difference is more pronounced farther away from the central axis of the tunnel (Figure 13.4b). Since we are primarily interested in the temperatures as measured in the axis of the clay bulkhead, and the temperature differences we are interested in explaining are on the order of 20\(^\circ\)C, we did not perform any 3D calculations for models which included fluid flow, which would have been computationally prohibitive. Moreover, since the 2D case overestimates the measured temperatures, the temperature discrepancy we are seeking will be more difficult to achieve than in 3D. Thus, our results remain robust.

### 13.2.2 Backfitted thermal parameters

In order to match measured temperatures, the thermal conductivity of the clay backfill was backfitted in MOTIF from \( k = 1.6 W/m/K \) to \( k = 0.26 W/m/K \) at day 420 of the
Figure 13.3: TSX thermal field assuming heat transfer by conduction only, using measured thermal parameters. Plotted are cross-sectional, edge and meshed boundary temperatures.
Figure 13.4: Comparison of calculated temperatures in a 2D and 3D model. a) Temperature profile along the axis of the clay backfill and bulkhead; b) Thermal profiles along the backfill/bulkhead interface through the entire height of the tunnel, where the temperature range plotted is much smaller than in a).
Figure 13.5: TSX temperature and velocity. All parameters are the same as in Figure 13.2, except for the thermal conductivity of the Clay Backfill which has been reduced from \( k = 1.6 \text{ W/m/K} \) to \( k = 0.26 \text{ W/m/K} \). The resulting temperatures at our four sampling points (see Figure 12.1) were: PZ20T: \( \sim 85^\circ C \); PSY47T: \( \sim 53^\circ C \); PZ5T: \( \sim 45^\circ C \); PZ6T: \( \sim 38^\circ C \) (also see Figure 13.6).
experiment. Using the identical model set up as that presented in Section 13.2.1, but substituting the backfitted $k$ in the clay backfill, we reproduced the backfitted MOTIF results (Figure 13.5 - compare with Figure 13.1b).

Thermal profiles for both the original and backfitted models are shown in Figure 13.6. Changing the backfill conductivity easily achieves the desired drop in temperatures as measured along the axis of the clay bulkhead. There is, of course, no physical reason for believing that the material properties of the backfill would have changed to that extent, especially since the concrete bulkhead would have had to have suffered the same fate. Instead, one or more of the physical changes outlined in Section 11.2 may have changed the effective thermal conductivity of the clay backfill or another domain.

### 13.3 Convective Case 1: Air bubbles in the sand chamber

We ran a model including occluded bubbles of air along the perimeter of the sand chamber, as suggested by Guo et al. (2005a) and Guo & Dixon (2009). The model parameters here were the same as those used in our base case, with the addition of a set of 1 cc air-filled bubbles (see Figure 13.7a) whose distribution is based on Figure 11.6. Because the viscosity of air is low and the flow is inertial, we could not model convection in these air pockets. Thus, the bubbles are simple conductors with the thermal conductivity of air ($k_{\text{air}} \sim 0.03 \text{ W/m/K}$) at these temperatures - we used the default temperature-dependent value from CM’s Materials Library. In reality, of course, the air would convect vigorously, increasing the effective thermal conductivity (and decreasing the thermal effect) of the small air bubbles.

Comparing Figures 13.2 and 13.7a, we see that the bubbles only had a very local effect, without any influence on the temperatures measured along the axis of the clay bulkhead. This is shown explicitly in 13.7b, where we see the local drop of $\sim 1^\circ C$ at the sand-backfill interface, which has entirely been diffused out 30 cm away at the backfill-bulkhead interface. The effect would be even less if we had been able to include
Figure 13.6: Thermal profiles for purely conductive heating in the clay domains using thermal conductivities for the clay backfill as measured \( (k = 1.6\, W/m/K) \) and adjusted in backfitting \( (k = 0.26\, W/m/K) \). Also marked (with x’s) are the locations of the three temperature sampling locations corresponding to PSY47T, PZ5T and PZ6T in the TSX. Chamber sand is heated by flow of hot water.
convection. The temperatures at the backfill-bulkhead interface (i.e. those measured by PSY47T) are identical to those measured at the same interface in the absence of bubbles.

13.4 Convective Case 2: Convective water-filled pockets

On decommissioning of the TSX, $1 - 10$ cc holes were found in the ‘low-density clay at the upstream key face’ (Guo et al., 2006), which we interpret to mean the rock/clay interface in the outer ring defined by the key cut into the granite to minimize flow through the EDZ. It was also suggested that such pockets may have formed throughout the clay bulkhead. We tested this by running models identical to our base case, with the addition of water-filled pockets in a number of locations in the clay backfill and bulkhead. In this suite of models, we assume there is no transfer of water between the water-filled pockets and the surrounding clay. We solved the calculation using CM’s parametric solver by gradually decreasing the viscosity of the convecting fluid.

In the model presented here we placed two $10 \times 10$ cm pockets along the axis of the clay seal, one in the backfill and one in the bulkhead, and one $10 \times 10$ cm at the contact between the bulkhead and the granite at the upper upstream key face. These represent pockets much larger than the size of the observed $10$ cc pockets. Figure 13.8a shows the resulting temperatures and velocity field for the two axial pockets. Figure 13.8b shows two temperature profiles, one through the two pockets, and the other just $25$ cm away in an area unaffected by the water-filled pockets, and which is identical to the profile for our base case (cf. Figure 13.2). The temperature re-distribution by the convecting fluid created a small local disturbance, which raised and lowered the temperatures up to by a maximum of $\sim 2^\circ C$ at the perimeter of the pocket and decreasing to a negligible amount $10 - 20$ cm up or downstream of it. This effect was greatest at higher temperatures.

Since all sampled temperatures along the bulkhead axis appeared to have been affected equally, the water pocket hypothesis would require a rather fortuitous arrangement of holes to have an observable effect (including in the concrete bulkhead on the other side
Figure 13.7: Temperature distribution in the TSX after formation of air bubbles in the sand chamber. a) Temperature field, showing the distribution of bubbles (compare with Figure 3.2). b) Thermal profiles along the sand/backfill interface (where no temperatures were sampled) and the backfill/bulkhead interface (where PSY47T was located at mid-height).
of the sand-filled chamber), and even then only accounts for a small fraction of the discrepancy.

The pocket at the upstream key face had a similar but muted effect due to the lower temperatures in that region. In addition, it is difficult to imagine a water pocket at the upstream key face having any effect on the temperatures at the central axis of the bulkhead.

One could imagine a network of interconnected 10 cc pockets of flowing water, perhaps along the joints between clay blocks. In order to affect the temperature sampling at PSY47T, PZ5T and PZ6T equally, however, such a network would have to be either pervasive throughout the bulkhead, or located upstream of the central axis of the bulkhead - i.e., in the backfill. Hence we tested the end-member case of a long 10 cm wide channel extending upwards and downwards to the granite in the center the clay backfill. If convection can whisk away heat to the granite heat sink above it, the effective thermal conductivity of the backfill could be reduced before reaching the temperature sampling points in the bulkhead.

The model shown in Figure 13.9 has the same set-up as our base case, with the addition of the extended (4 × 0.1 m) water pocket in the clay backfill. The water pocket does appear to advect incoming heat upwards to the granite to a small degree. However, the accompanying temperature drop in the bulkhead is negligible. In addition, the small pockets and flow channels found in the clay seal on decommissioning were not connected in this way (Martino et al., 2006).

13.5 Convective Case 3: Microfissures in the Sand Chamber

The final idea proposed by the TSX modeling team for the discrepancy between the predicted and measured temperatures was the formation of small microcracks or fissures in the chamber sand (Guo et al., 2005b). Fissures would have directed the flow of heated water through subsections of the sand chamber, leaving heat transport in large
Figure 13.8: Convecting water pockets in the clay backfill and bulkhead. a) Temperature field, showing fluid flow in the two water pockets in the clay backfill and bulkhead along the axis. b) Thermal profiles from the sand chamber to past the second pocket through the mid-point of each pocket.
Figure 13.9: Convection water in a long wide ‘fissure’ representing a series of small connected pockets of water. Notice the heat advected to the top of the fissure where it is absorbed by the granite heat sink. It should be noted that this model was not stable at realistic viscosities for water; the model shown here is for a fluid with $\sim 20$ times $\eta_{\text{water}}$. Although this scenario is neither realistic nor effective at reducing heat in the bulkhead, it is fun to model from a fluids point of view.
sections of the chamber to conduction alone. Such fissures may have formed early in the pressurization of the chamber and been amplified by the loss of chamber hydraulic pressure at day 51 of the experiment, which left the chamber depressurized for several hours while the broken valve was fixed. Loss of hydraulic pressure would have facilitated the collapse of sand into more or less consolidated pieces. Fissures would have been kept open and interconnected where and when the vigour of convection was greatest; therefore, initially unimportant fissures would become increasingly active with rising temperatures and pressures in areas where the fluid velocity was greatest. Nevertheless, we will show that they need have only been as wide as $0.5 - 1\, mm$, spaced $10 - 100\, cm$ apart; such small features may have been missed (or destroyed) during decommissioning.

As with the results of Guo & Dixon (2009) and others, our models do not explicitly reproduce the flow of water through microfissures, except in the most coarse fashion as we did in Section 13.4. The resolution needed to resolve a series of water-filled fissures $10^{-2} - 10^{-3}\, m$ in size was beyond our computational power.

An alternative approach is to model flow through fissures or cracks using the Brinkman equations for flow through porous media, representing flow through fissures using an equivalent (lowered) permeability. Because the Brinkman equations are essentially a Navier-Stokes formulation where the viscosity is reduced by the friction between the flowing media and the pores of the solid matrix, they are much more stable than the regular Navier-Stokes equations except at very low permeability.

### 13.5.1 Equivalent conductivity approximation

We consider the simplest case, where the fluid flows through a homogeneously distributed series of parallel cracks (here, in the vertical direction). We begin with an equation for the equivalent permeability for laminar flow through two parallel plates (Poiseuille Flow). Comparison with Darcy’s law for viscous flow through porous media under a gradient in pressure yields an equivalent permeability for flow through a network of parallel fissures.

Following the formulation of Turcotte & Schubert (2002), we begin with the equation of motion for non-inertial flow between two plates
Figure 13.10: Definition of parameters used in the equivalent permeability derivation.

\[
\frac{d\sigma}{dx} = \frac{dp}{dz} \tag{13.1}
\]

where \(\sigma\) is shear stress, \(x\) and \(z\) are defined in Figure 13.10, and \(\frac{\partial p}{\partial z}\) is the vertical pressure gradient in the channel. By definition

\[
\sigma = \eta \frac{du}{dx} \tag{13.2}
\]

where \(\eta\) is the viscosity of the fluid and \(u\) is velocity. Hence the velocity is defined by

\[
\eta \frac{d^2u}{dx^2} = \frac{dp}{dz} \tag{13.3}
\]

Integrating this equation and applying no-slip boundary conditions (\(u = 0\) at the walls) yields the channel velocity
\[ u = \frac{1}{2\eta} \frac{dp}{dz} (x^2 - 2ax) \] (13.4)

where 2a is the width of the channel (see Figure 13.10). The mean fluid velocity \( \bar{u} \) is therefore

\[ \bar{u} = \frac{1}{2a} \int_0^{2a} \frac{dp}{2\eta} dz (x^2 - 2ax) dx \] (13.5)

which gives

\[ \bar{u} = -\frac{(2a)^2 dp}{12\eta} \frac{dz}{dz} \] (13.6)

The flow rate \( q \) through a fissure of length \( L \) is defined as

\[ q = (2a)L\bar{u} = -\frac{(2a)^3 L dp}{12\eta} \frac{dz}{dz} \] (13.7)

and the flux through an area of length \( L \) and which contains fissures separated by a distance \( A \) is defined as

\[ J = \frac{q}{LA} = -\frac{(2a)^3 dp}{12\eta A} \frac{dz}{dz} \] (13.8)

Comparing this with a one-dimensional form of Darcy's law

\[ J = -\frac{\kappa dp}{\eta dz} \] (13.9)

we can define an equivalent permeability for a system of fissures separated by a distance \( A \) as

\[ k = \frac{(2a)^3}{12A} \] (13.10)

For example, an effective permeability of \( 10^{-9} \text{m}^2 \) represents flow through a series of 1 mm fissures spaced \( \sim 8 \text{cm} \) apart. We assume \( \leq 1 \text{mm} \) fissures for all our models, and calculate the separation distance accordingly. Larger fissures might have been less easily missed or destroyed on decommissioning.

It should be noted that this approximation is valid for flow through fissures in an otherwise impermeable matrix. In our models, we apply this approximation for areas within larger permeable domains. However, the permeability of the sand chamber and clay/sand mixtures is 3 to 7 orders of magnitude smaller than the effective permeability
needed to reproduce the measured temperatures, therefore this approximation remains valid.

13.5.2 Results

We ran this suite of models using Comsol’s Parametric solver, gradually lowering the permeability in the sand chamber (i.e. increasing the density of fissures) for numerical stability. Except for this change, all chamber fissure models had the same parameters as our base case. All other domains were heated by conduction only.

Our first calculation was for a homogeneously distributed series of fissures throughout the entire sand chamber. Each calculation began with a permeability of $10^{-12} \text{m}^2$ (the measured permeability of the chamber sand was $6.25 \times 10^{-12} \text{m}^2$), which was decreased it to $10^{-8} \text{m}^2$. For $\leq 10^{-9} \text{m}^2$ the flow was similar to our base case; for higher permeabilities, it began to segregate into a strong unidirectional flow in the region between the inlet and outlet, and an increasingly complex return flow beyond this region (Figure 13.11a). Because of this complex flow, the outer edge of the chamber sand were still heated by convection, and the effective thermal conductivity sand chamber remained relatively high throughout (reaching its lowest value at $\sim 1.5 \times 10^{-9} \text{m}^2$ - see Figure 13.11b). As a result, the temperatures measured in the axis of the bulkhead remained higher than observed.

However, it is plausible that fissures created by the malfunction at day 51 of the experiment would have settled and closed as the hydraulic pressure was increased, unless they were sustained by vigorous flow of the heated water. In addition, the brief change in pressure at day 51 would have been greatest in areas of higher flow velocities, focusing the opening of fissures in the region between the inlet and outlet. It is reasonable to assume, then, that fissures would more likely have been found in the direct path between the inlet and outlet of the heated water.

To test this, we delimited an area connecting the heater inlet to the heater outlet, and lowered the permeability in this area only. In other words, we assumed that the permeability outside this area remained at the measured permeability of the chamber sand. The change in chamber flow with increasing fissure density is shown in Figure 13.12. The effect of increasing fissure density on the sampled temperatures in the bulkhead is
Figure 13.11: Fluid flow through fissures uniformly distributed in the Sand Chamber. a) Temperature (colour) and velocity field (arrows); the horizontal black line shows where the thermal profiles are measured; b) Thermal profiles through the chamber, backfill and bulkhead (see black line in (a)) for three different permeabilities.
Figure 13.12: Fissure flow from the heated water inlet to the outlet. The boundary of the fissured area is marked by vertical lines at the edges of the heater inlet and outlet. Inside this region, permeability increases from A \((10^{-11} \text{ m}^2)\) to D \((10^{-8} \text{ m}^2)\) by an order of magnitude in each part of the figure, representing an increase from 1 \(\text{mm}\) fissures every 8 m in A to \(\sim 0.5 \text{mm}\) fissures every m in D. The area outside the fissured area has the measured permeability of the chamber sand \((6.25 \times 10^{-12} \text{ m}^2)\).
shown in Figure 13.13.

Our results show that an equivalent permeability of $10^{-9} \text{ m}^2$ (created by 1 mm fissures every 8 cm, or $\sim 2$ mm fissures every m) in the area directly connecting the sand chamber heater inlet to the outlet reduces the temperature measured at PSY47T (at the backfill/bulkhead interface) by $\sim 18^\circ C$. The discrepancy between the temperatures predicted by MOTIF calculations and those measured during the operation of the TSX at PSY47T was $\sim 20^\circ C$ (Guo & Dixon, 2009). Since the MOTIF calculations appear to have predicted temperatures $\sim 2\text{–}3^\circ C$ higher than ours, our models suggest that fissure flow between the inlet and outlet heaters was the main cause of the discrepancy.

Thus, as predicted by Guo et al. (2005b), a large part of the sand chamber transferred heat to the seals mainly by conduction, while convective flow was limited to the two regions connecting the inlets and outlets. Moreover, this would have affected both seals equally, as there is no reason to suspect fissures to have formed between one of the inlet/outlet water heater pairs more than the other.

### 13.6 Summary

We have tested three hypotheses to explain the discrepancy between the measured and observed temperatures in the clay and concrete seals tested at AECL’s Tunnel Sealing Experiment in Whiteshell, Manitoba. These are: 1) the formation of air bubbles in the heated sand chamber due to the dissolution of air from the heated water; 2) the formation of small pockets of water in the clay bulkhead; and 3) the formation of microfissures in the sand chamber itself due to a number of hours of pressure drop on day 51 of the experiment. We find that the first two may produce small local variations in temperature, but are unlikely to have produced a temperature drop of up to $\sim 20^\circ C$ on both sides of the sand chamber and throughout each of the clay and concrete seals. The third hypothesis appears to be able to explain the entire discrepancy, if the flow of heated water through microfissures is limited to the parts of the sand chamber directly connecting the inlet and outlet heaters. This also explains why the temperatures measured in the granite (at EXT2-2T to EXT2-6T) matched the predicted temperatures, as these sensors were
Figure 13.13: Temperatures measured at PSY47T (triangles), PZ5T (circles) and PZ6T (squares) for increasingly permeable flow between the inlet and the outlet.
located directly below one inlet heater (Figure 11.3). Since flow through fissures should reduce total heat transfer to the sand chamber, perhaps one way to test whether this type of fissure flow occurred would be to see if the water flowing out of the chamber was slightly hotter than expected, or if less power than expected was needed in the heating system. However, depending on the amount of heat lost to the rock from the inlet/outlet piping, it is not clear that this method would be conclusive.

Our results attempt to resolve the predicted and measured temperatures at day 420 of the experiment - that is, immediately prior to decommissioning. Close inspection of Figure 11.5a reveals that the discrepancy grew with time after each increase in heater temperature. In other words, the response of the system to changes in temperature was not immediate. If the cause was microfissures in the chamber sand as our models suggest, the response time would simply be the time for existing fissures to broaden or connect, or new fissures to form, in response to the increased vigour of convection resulting from higher temperatures. Once set, microfissures may not have been stable features, but evolved under small changes in the convective pressures of the fluid.

13.7 Conclusion

The Tunnel Sealing Experiment appears to have been a success overall, in the sense that the two seals successfully limited water seepage from the Sand Chamber. This is especially convincing considering that the high temperatures and pressures imposed during the TSX are much greater than any predicted pressures and temperatures in the real application of these seals for Deep Geological Repositories for Nuclear Waste.

The discrepancy between the predicted and measured temperatures was a concern, since a physical cause was suspected which may or may not have impacted the future application of similar clay and concrete seals. Our results suggest that the physical cause which created the problem will not exist during the eventual use of such seals. This is because neither the sand chamber, the forced flow of water, nor the damaged valve in the pressurizing system (whose failure at day 51 was at the root of the problem) will exist during the operation of a DGR. Therefore, if our conclusions are correct, the major
unresolved problem with the TSX should not be of concern for the implementation of clay and concrete bulkheads in well-chosen geological nuclear waste repositories.
Part IV

Appendix
A. Derivation of Model Geotherms

The equilibrium thermal profile satisfies the ordinary differential equation (Turcotte & Schubert (2002))

\[ k \frac{d^2T}{dy^2} = -H(y) \] (13.11)

where \( T \) is temperature (in °C), \( k \) is the thermal conductivity, \( H(y) \) is the distribution of heat with depth, and \( y \) is positive downwards. For a half-space with temperature \( T(y = 0) = T_0 \) and heat flux \( q = q_0 \) defined at at the surface, Equation 13.11 is integrated twice to give \( T(y) \)

\[ T(y) = T_0 + \frac{q_0}{k} y - \frac{H}{2k} y^2 \] (13.12)

Since in our model we approximate \( H \) as constant with depth in the granitic layer only, we define \( q_0 = q_m + HD \), where \( q_m \) is the heat flow from the mantle, and \( D \) is the vertical extent of the granitic layer. In our case, we take \( T(y = 0) = 0 \). We divide our system piecewise into 3 parts as shown in Figure 2.3, and calculate \( T(y) \) in each part as follows (see Figure 2.4):

\( 0 < y < y_1 \):

\[ T(y) = \frac{q_m + HD}{k} y \] (13.13)

\( y_1 < y < y_2 \):

\[ T(y) = \frac{q_m + HD}{k} y_1 + \left( \frac{q_m + HD}{k} (y - y_1) - \frac{H(y - y_1)^2}{2k} \right) \] (13.14)

\( y_2 < y < y_3 \):

\[ T(y) = \frac{q_m + HD}{k} y_1 + \frac{(q_m + HD)D}{2k} - \frac{HD^2}{2k} + \frac{q_m(y - y_2)}{k} \] (13.15)
where \( D = y_2 - y_1 \), and \( y_1, y_2 \) and \( y_3 \) are 10 km, 25 km, and 35 km respectively. For each calculation, the initial temperature distribution is 0 in the top layer, and equal to the equilibrium temperature in the absence of the top layer in the bottom two layers.

In practice, this meant that for each set of \( q_m \) and \( H \), we calculated the initial thermal profile below 10 km using equations 13.14 and 13.15 and setting \( T(y_1) = 0 \), and fit it to a 5th order polynomial which we input into Thermax2d, attached to a 0 function in the top 10 km (using the Matlab function \( y = \text{sign}(x) \)). This assumed that the interface between the first and second layers was flat (i.e. we ignored the sinusoidal interface), a small approximation which appeared to be the only tractable way to avoid a temperature discontinuity between the two layers.

B. A note on finite strain theory

Typically, discussions on finite strain theory found in most structural mechanics or geodynamic textbooks centers on deriving the finite strain tensor. As it turns out, this is in fact not very useful in terms of finding measurable quantities. Performing the derivation will show why this is the case. The derivation of the more useful (and simpler) quantity \( \epsilon \) (linear strain) will also be presented, and is the one used in the strain results presented in Chapter 4.

The deformation tensor in the Lagrangian frame of reference is (Means, 1976; Ranalli, 1995; Turcotte & Schubert, 2002; Robin, 2009):

\[
\begin{pmatrix}
  x \\
  y
\end{pmatrix} =
\begin{pmatrix}
  \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} \\
  \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y}
\end{pmatrix}
\begin{pmatrix}
  X \\
  Y
\end{pmatrix}
\]

or

\[
x_i = \frac{\partial x_i}{\partial X_j} X_j = V_{ij} x_j \tag{13.16}
\]

where \((x,y)\) are the current coordinates, and \((X,Y)\) are the original coordinates of a material point, and the Einstein summation convention is used. In the Eulerian frame, we have:
\[
\begin{pmatrix}
X \\
Y
\end{pmatrix} = \begin{pmatrix}
\frac{\partial X}{\partial x} & \frac{\partial X}{\partial y} \\
\frac{\partial Y}{\partial x} & \frac{\partial Y}{\partial y}
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
\]

or

\[X_i = \frac{\partial X_i}{\partial x_j} x_j = W_{ij} x_j\] (13.17)

Since derivatives in Thermax2d are always with respect to the current coordinates \(x_i\), the rest of this discussion will be restricted to the Eulerian case. From Equations 13.16 and 13.17 we see that the Eulerian deformation tensor is the inverse of the Lagrangian deformation tensor \((UV = 1)\).

Following Ranalli (1995), the change in length of a segment of line from \(ds_0^2 = dX_i dX_i\) to \(ds^2 = dx_i dx_i\) is given by

\[ds^2 - ds_0^2 = dx_i dx_i - dX_i dX_i = \delta_{jk} dx_j dx_k - \frac{\partial X_i}{\partial x_j} \frac{\partial X_i}{\partial x_k} dx_j dx_k = 2 \varepsilon_{jk} dx_j dx_k\] (13.18)

giving a definition of the finite strain tensor as

\[\varepsilon_{jk} = \frac{1}{2} \left( \delta_{jk} - \frac{\partial X_i}{\partial x_j} \frac{\partial X_i}{\partial x_k} \right)\] (13.19)

or

\[E = \frac{I - W^T W}{2}\] (13.20)

We can reformulate \(E\) in terms of displacement \(u_i = x_i - X_i\), and using the fact that \(\frac{\partial x_i}{\partial x_j} = \delta_{ij}\):

\[
\frac{\partial X_i}{\partial x_j} \frac{\partial X_i}{\partial x_k} = \left( \delta_{ij} - \frac{\partial u_i}{\partial x_j} \right) \left( \delta_{ik} - \frac{\partial u_i}{\partial x_k} \right) = \delta_{ij} - \frac{\partial u_j}{\partial x_k} - \frac{\partial u_k}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_k}\] (13.21)

Hence, in the Eulerian framework, the strain tensor is

\[E_{jk} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_k} \right)\] (13.22)
For the two dimensional case, filling in the components of the displacement gradient tensor

\[ U_{i,j} = \frac{\partial u_i}{\partial x_j} = \frac{\partial x_i - \partial X_i}{\partial x_j} \]  

(13.23)

defines the components of finite strain as

\[ E_{xx} = 1 - \frac{\partial X}{\partial x} - \frac{1}{2} \left[ \left(1 - \frac{\partial X}{\partial x}\right)^2 + \left(- \frac{\partial Y}{\partial x}\right)^2 \right] \]  

(13.24)

\[ E_{yy} = 1 - \frac{\partial Y}{\partial y} - \frac{1}{2} \left[ \left(1 - \frac{\partial Y}{\partial y}\right)^2 + \left(- \frac{\partial X}{\partial y}\right)^2 \right] \]  

(13.25)

\[ E_{xy} = \frac{1}{2} \left[ -\frac{\partial X}{\partial y} - \frac{\partial Y}{\partial x} + \left(1 - \frac{\partial X}{\partial x}\right) \left(\frac{\partial X}{\partial x}\right) + \left(\frac{\partial Y}{\partial x}\right) \left(1 - \frac{\partial Y}{\partial y}\right) \right] \]  

(13.26)

\[ E_{xy} = E_{yx} \]  

(13.27)

This is, therefore, the finite strain tensor as defined in such classic texts as Means (1976), Ranalli (1995) and Turcotte & Schubert (2002). The physical interpretation of \( E \), however, is of limited value for most finite strain applications (Robin, 2009). For example, if the off-diagonal elements are set to zero (\( E_{xy} = E_{yx} = 0 \), making the x-axis a principal axis), then

\[ E_{xx} = U_{xx} + \frac{U_{xx}^2}{2} \]  

(Robin, 2009). For small or infinitesimal strain, the second order terms are dropped, and

\[ E_{xx} = U_{xx} = 1 - \frac{\partial X}{\partial x} = 1 - W_{xx} = 1 - S_x \]

where \( S_x \) is the measurable quantity called stretch, here in the x direction. (In the Lagrangian frame, \( E_{xx} = U_{xx} = \frac{\partial X}{\partial x} - 1 = S_x - 1 \). Hence, the strain tensor is of interest in the case of infinitesimal strain, and is present in numerous engineering textbooks. However, for finite strain, important in geological applications, \( E_{xx} \) is related to stretch, but do not actually represent measurable quantities.
This is further illustrated for large strains. In the Eulerian framework, as $dx_j$ tends to $\infty$, \( \frac{\partial X_i}{\partial x_j} = W_{ij} \) tends to 0 and $E = \frac{I - W^TW}{2}$ tends to 0.5 (this may be what was plotted in the strain figures of Mareschal & West (1980), who get a maximum strain of 0.5 at a point in the evolution of the diapir where our models give strains of 5-10). This not the case in the Lagrangian framework (where $E = \frac{W^TW-I}{2}$), but even then the finite strain tensor remains no more physical meaningful.

The second order terms included for large or finite strains account for normal stretch in the diagonal terms, and define the angle between two initially orthogonal lines in the off-diagonal terms (Figures B,C). For that reason, and given the limitations outlined above, the finite strain tensor may be of interest only in special cases, such as in the case of small strains with large rotations (P.-Y. Robin, personal communication).

Instead, what is typically of interest is the axial ratio of a strain ellipse, or the stretch ratio

$$
R = \frac{1 + \varepsilon_1}{1 + \varepsilon_2} = \frac{S_1}{S_2}
$$

where $\varepsilon$ is linear strain, and $S_{1,2} = \frac{L_{1,2}'}{L_{1,2}} = 1 + \varepsilon_{1,2}$ are the stretch ratio measured in the principal directions of strain (Figure A). The principal directions are the eigenvalues of the symmetric deformation tensor. Thus, mapping strain is essentially an exercise in finding the symmetric deformation tensor.

Finite deformation is rarely symmetric, but can be represented as the product of symmetric strain and rotation through an angle $\omega$:

$$
W = R(\omega)W^s = \begin{pmatrix}
\cos(\omega) & \sin(-\omega) \\
\sin(\omega) & \cos(\omega)
\end{pmatrix} W^s
$$

where $W^s$ is the symmetric strain tensor.
Therefore

\[ W^s = R(-\omega)W \]  

(13.29)

Equating the off-diagonal elements \( W_{xy}^s = W_{yx}^s \)

\[
\cos \omega \cdot W_{yx} - \sin \omega \cdot W_{xx} = \cos \omega \cdot W_{xy} + \sin \omega \cdot W_{yy}
\]

(13.30)

defines \( \omega \) as:

\[
\tan \omega = \frac{W_{yx} - W_{xy}}{W_{xx} + W_{yy}}
\]

(13.31)

As mentioned above, \( \varepsilon_{1,2} \) are the deviations of the axes of the strain ellipse from 1 (a circle). The strain ellipse is defined in the direction for which there is no shear strain. Hence, we must find the axes in which the shear component of strain is zero, which are principal components or eigenvectors of \( W^s \).

Solving for the roots of

\[
|W^s - wI| = 0
\]

gives principal components

\[
w_{1,2} = \frac{1}{2}[(W_{xx}^s + W_{yy}^s) \pm \sqrt{(W_{xx}^s - W_{yy}^s)^2 + 4(W_{xy}^s)^2}] 
\]

(13.32)

and the characteristic equations

\[
\begin{pmatrix} W_{xx}^s & W_{xy}^s \\ W_{xy}^s & W_{yy}^s \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = w_{1,2} \begin{pmatrix} a \\ b \end{pmatrix}
\]

where \( a = \cos(\theta) \) and \( b = \sin(\theta) \). The principal directions are therefore

\[
\tan \theta_1 = \frac{w_1 - W_{xx}^s}{W_{xy}^s} = \frac{W_{xy}^s}{w_{max} - W_{yy}^s}
\]

(13.33)

and

\[
\tan \theta_2 = \frac{w_2 - W_{xx}^s}{W_{xy}^s} = \frac{W_{xy}^s}{w_{min} - W_{yy}^s}
\]

(13.34)

It should be noted that most text books present the principal directions of strain or stress as \( \tan(2\theta) = 2E_{xy}/(E_{xx} - E_{yy}) \) giving two principal directions \( \theta \) and \( \theta \pm \pi/2 \) Ranalli (1995); Turcotte & Schubert (2002). However, care must be taken to make sure the tan function is in the correct quadrant, which can be dealt with using a tangent
function such as the `atan2(Y,X)` function in Matlab. In general, however, the formulation given in (17) and (18) is less cumbersome. This must also be taken into account when solving for $\omega$.

In the Eulerian framework, the symmetric deformation tensor

$$
\begin{pmatrix}
  w_{\text{min}} & 0 \\
  0 & w_{\text{max}}
\end{pmatrix}
$$

defines the long and short axes of the finite strain ellipse (in the Lagrangian frame the symmetric deformation tensor $V^s$ is $(W^s)^{-1}$).

$$
R = \frac{1 + \varepsilon_1}{1 + \varepsilon_2} = \frac{S_1}{S_2} = \frac{w_{\text{max}}}{w_{\text{min}}}
$$

(13.35)

It is now trivial to extract $\varepsilon_1$ and $\varepsilon_2$ from $w$. Note that since we are principally interested in $w_{\text{max}} = 1 + \varepsilon_1$, we must be careful to use $\theta_2$ or $\theta_1 + \pi/2$ as the principal direction in the Eulerian framework, unlike in the Lagrangian framework. However, unlike in the Eulerian case, the derivatives in the Lagrangian framework are with respect to the original un-rotated configuration, and the principal directions of $U^s$ in the final deformed state must be adjusted to $\theta_2 + \omega$ if we are interested in the strain ellipse in the final state.

Finally, since volume is conserved, $w_{\text{max}}w_{\text{min}} = (1 + \varepsilon_1)(1 + \varepsilon_2) = 1$. 
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