

IMPERIAL COLLEGE LONDON

Investigating melt emplacement, storage, and
evolution in the shallow crust beneath
active volcanic centres using thermo-mechanical
modelling of repetitive sill intrusions

Author:

Katarina Roele

Supervisors:

Professor Joanna Morgan

Professor Matthew Jackson

Dr Michele Paulatto

Submitted in part fulfilment of the requirements for the degree of

Doctor of Philosophy in Geophysics

at The Imperial College of Science, Technology, and Medicine

October 13, 2018

Copyright Declaration

The copyright of this thesis rests with the author and is made available under a Creative Commons Attribution Non-Commercial No Derivatives Licence. Researchers are free to copy, distribute, or transmit the thesis on the condition that they attribute it, that they do not use it for commercial purposes and that they do not alter, transform, or build upon it. For any reuse or redistribution, researchers must make clear to others the licence terms of this work.

Katarina Roele

Department of Earth Science and Engineering

Imperial College London

October 13, 2018

Declaration of Originality

I declare that this thesis titled, **Investigating melt emplacement, storage, and evolution in the shallow crust beneath active volcanic centres using thermo-mechanical modelling of repetitive sill intrusions**, and the work presented in it are my own, performed under the supervision of Professor Joanna Morgan, Professor Matthew Jackson, and Dr Michele Paulatto at the Department of Earth Science and Engineering, Imperial College London. All published and unpublished material used in the thesis has been given full acknowledgement. This thesis has not been previously submitted in whole or in part for a degree or any other qualification at this University or any other institution.

Katarina Roele

Department of Earth Science and Engineering
Imperial College London

October 13, 2018

Abstract

Understanding the spatial and temporal evolution of melt distribution in the crust is crucial in providing insight into the development of sub-volcanic crustal stratigraphy and composition. A quantitative model of heat and mass transport through a compacting, highly crystalline crustal mush created through repetitive intrusions of is presented. In contrast with previous static models of heat transfer in the crust, it is found that realistic, intermediate emplacement rates are capable of forming persistent high melt fractions in the shallow crust. The structure of the high melt fraction volumes consists of crystal-poor lenses within a crystalline matrix, where the lenses accumulate through segregation at the top of the system, bounded by the solidus isotherm. Melt distributions predicted by thermo-mechanical modelling provide evidence for the emerging concept of mushmatism and its dominant role in the lifecycle of shallow crustal magma reservoirs. Results of the thermo-mechanical model are benchmarked against those of static models and used to estimate velocities across sub-volcanic systems. Velocity anomalies are estimated using a combination of Karato's method and Berryman's self-consistent approach. Comparison between the velocity profiles estimated from the thermo-mechanical model and those developed using a static model to match recorded data from the SEA-CALIPSO seismic experiment show that lower emplacement rates of only 10 mmpa, compared with 750 mmpa in the static model, are required to produce the same velocity signature when melt segregation is accounted for. Resulting velocity models are used to generate synthetic seismic data for a full waveform inversion (FWI) using a starting model recovered from a synthetic travel-time inversion produced with the software package tomo2d. The resulting velocity model recovered using FWI investigates its potential use in recovering the fine-scale structure of sub-volcanic plumbing systems and the maximum inversion frequency at which a full-scale 3D FWI at active volcanic centres could be implemented.

Acknowledgements

I would like to thank my supervisors; Professor Joanna Morgan, Professor Matthew Jackson, and Dr. Michele Paulatto for their continued help and guidance throughout my PhD. In particular Michele for joining on to the project late in the day to help out and for giving me so much of his time - you are an excellent teacher! In addition I would like to thank Dr Ian Bastow for being an excellent mentor and always providing support when needed. Thanks also go to Peter Allison for being so supportive and to Mike Warner for helping me through the last hurdles. Finally, thank you to my family and friends for their help over the last few months, particularly Will Haining for editing the final draft.

Contents

Title Page	i
Copyright Declaration	ii
Declaration of Originality	iii
Abstract	iv
Acknowledgements	v
Table of Contents	viii
List of Figures	xi
List of Tables	1
1 Introduction	2
1.1 Motivation	3
1.2 Aims and objectives	4
1.3 Structure of this thesis	4
2 Literature Review	6
2.1 Thermo-mechanical modelling	7
2.2 Calculating elastic moduli	9
2.3 Seismic inversion	11
2.4 Conclusion	15
3 Thermo-mechanical Model - Description and Benchmarking	16
3.1 Background	17
3.2 Early thermal modelling	22

3.3	Melt segregation and reactive flow	28
3.4	Method	31
3.5	Benchmark: one dimensional column	33
3.6	Benchmark: deep crustal hot zones	37
3.7	Benchmark: thermo-mechanical modelling	43
3.8	Grid resolution study	47
3.9	Modelling carried out	51
3.10	Results	51
3.11	Discussion	64
3.12	Conclusion	65
4	Estimating Seismic Velocities	67
4.1	Background	68
4.2	Method	75
4.3	Results	85
4.4	Discussion	100
4.5	Conclusion	102
5	Modelling the Shallow Crust	104
5.1	Background	105
5.2	Background of the study area	107
5.3	Method	117
5.3.1	Numerical modelling	117
5.3.2	Seismic travel-time tomography	117
5.3.3	Parameter testing and benchmarks	120
5.3.3.1	Cooling post intrusion	120
5.3.3.2	Constant volume	121
5.3.3.3	Constant run time	121
5.3.3.4	Minimum emplacement rate	122
5.4	Results	123
5.4.1	Cooling post intrusion	128
5.4.2	Constant volume	134
5.4.3	Constant run time	139
5.4.4	Minimum emplacement rate	143
5.5	Discussion	151

5.6	Conclusion	155
6	Travel Time Tomography and Full Waveform Inversion Comparison at Montserrat	158
6.1	Background	159
6.2	Method	162
6.3	Results	166
6.4	Discussion	172
6.5	Conclusion	174
7	Conclusion and Future Work	176
7.1	Summary and conclusions	177
7.2	Future work	181
	Appendix	192
	Bibliography	193

List of Figures

3.1	Comparison of traditional magma chamber with mush column.	22
3.2	The Bowen series.	24
3.3	Model domain adapted from Annen (2009).	25
3.4	Depiction of melt segregation adapted from Richter and McKenzie (1984).	30
3.5	Benchmarking thermo-mechanical model velocity results against those of Richter and McKenzie (1984).	36
3.6	Depiction of a volcanic plumbing system.	39
3.7	Benchmark against thermal model of Annen et al. (2006)	42
3.8	Benchmark against the 1D thermo-mechanical results of Jackson et al. (2018).	46
3.9	Grid resolution study for the temperature and melt fraction calculations in the thermo-mechanical model.	49
3.10	Dependence of the thermo-mechanical model results on the time-step used.	50
3.11	Comparison at emplacement rate of 100mmpa via under accretion.	54
3.12	Comparison at emplacement rate of 100mmpa via over accretion.	55
3.13	Comparison at emplacement rate of 25mmpa via over accretion at 115ka.	57
3.14	Comparison at emplacement rate of 25mmpa via over accretion at 300ka.	58
3.15	Comparison at emplacement rate of 10mmpa via over accretion at 600ka.	60
3.16	Comparison at emplacement rate of 10mmpa via over accretion at 1.51Ma.	62
3.17	Comparison at emplacement rate of 25mmpa via over accretion at 300ka.	63
4.1	Schematic diagram of the Kuster-Toksöz model for calculating elastic moduli.	74
4.2	Schematic diagram of the Berryman model for calculating elastic moduli.	75
4.3	Benchmarking the high-frequency solution against results of Paulatto et al. (2012). . .	91
4.4	Benchmarking the low-frequency approximation against results of Paulatto et al. (2012). .	92
4.5	Test on the least squares convergence for the velocity approximation.	93

4.6	1D velocity and bulk modulus results for corresponding temperature and melt fraction profiles using a purely thermal model and low-frequency approximation.	94
4.7	1D velocity and bulk modulus results for corresponding temperature and melt fraction profiles when melt segregation is accounted for in the thermo-mechanical model and the low-frequency approach is used.	95
4.8	Melt fraction and silica content results for the thermo-mechanical model.	96
4.9	a) 2D velocity profile and b) 2D velocity anomaly derived from the 1D purely thermal model with the low-frequency approximation.	97
4.10	a) 2D velocity profile and b) 2D velocity anomaly derived from the 1D thermo-mechanical model with the low-frequency approximation.	98
5.1	SEA-CALIPSO experimental geometry, Montserrat.	111
5.2	Travel time tomography inversion along 2D transect at Montserrat from Paulatto et al. (2012)	114
5.3	Ray density along horizontal slice at Montserrat calculated by Paulatto et al. (2012) .	115
5.4	Temperature and melt fraction estimates calculated from the SEA-CALIPSO 2D p-wave velocity model by Paulatto et al. (2012)	116
5.5	Comparison between purely thermal results of the thermo-mechanical model and those of Paulatto et al. (2012)	125
5.6	Comparison between results of the thermo-mechanical model with melt segregation and those of Paulatto et al. (2012)	126
5.7	Overlay of the original temperature and melt fraction results from the thermo-mechanical model on the estimated velocity profile.	127
5.8	1D velocity and bulk modulus results for corresponding temperature and melt fraction profiles after 60 ka of cooling.	129
5.9	1D velocity and bulk modulus results for corresponding temperature and melt fraction profiles after 120 ka of cooling.	130
5.10	1D silica content results through the centre of the pluton after cooling for a) 60 ka and b) 120 ka	131
5.11	Comparison of 2D results for 60 ka and 120 ka of cooling post final sill emplacement. .	133
5.12	Comparison of 2D results for the same emplaced volume at rates of 75 mmpa and 7.5 mmpa.	135
5.13	1D temperature, melt fraction, velocity, and bulk modulus results for the same emplaced volume at 75 mmpa	136

5.14	1D temperature, melt fraction, velocity, and bulk modulus results for the same emplaced volume at 7.5 mmpa.	137
5.15	1D silica content results through the centre of the pluton during emplacement at a rate of 7.5 mmpa	138
5.16	Comparison of 2D results for emplaced volumes of 3 km and 2 km at emplacement rate of 750 mmpa.	140
5.17	1D results for emplaced volume of 2 km at emplacement rate of 750 mmpa.	141
5.18	1D temperature, melt fraction, and silica content results for emplaced volumes of 3km and 2.1km.	142
5.19	Comparison of 2D results for sills 100 metres thick emplaced at 10 mmpa at 5 km and 3 km depth.	144
5.20	Temperature and melt fraction results of the thermo-mechanical model superimposed on the final 2D velocity profile.	147
5.21	Comparison between results of the thermo-mechanical model and those of Paulatto et al. (2012)	148
5.22	1D temperature, melt fraction, velocity, and bulk modulus results the final thermo-mechanical model.	149
5.23	1D temperature and melt fraction results comparison for thermal and thermo-mechanical model.	150
6.1	2D velocity profile interpolated from the tomo2d travel time tomography package. . .	165
6.2	a) Start, b) recovered, and c) true models from tomo2d.	166
6.3	a) Start and b) true models for FWI.	168
6.4	Recovered models from a) tomo2d and b) FWI.	169
6.5	Recovered velocity models from FWI run to 4, 6, 10, and 17.5 Hz.	171
7.1	Comparison of 2D thermo-mechanical model results with Annen (2009).	183
.2	Schematic of the temperature diffusion gradient to be solved. Drawing is not to scale. The solid line shows the geotherm at 50 Kkm^{-1} while the dashed line shows the gradient produced by the emplacement of heat as sills after 23 ka residence time.	186
.3	Schematic of the analogous diffusion gradient problem to be solved. Drawing is not to scale.	187
.4	Schematic of the analogous diffusion gradient problem being solved. Drawing is not to scale.	191

List of Tables

3.1	Temperature and melt fraction relationship for the binary eutectic phase diagram used.	40
3.2	Melting relationship for Annen et al. (2006).	40
3.3	Parameters used to benchmark against Annen et al. (2006).	41
3.4	Parameters used to benchmark against Jackson et al. (2018).	43
4.1	Coefficients for determining elastic moduli taken from Berryman (1980b)	82
4.2	Parameters used to produce figures 3.6 - 3.10 using inputs from Paulatto et al. (2012).	99
5.1	Parameters used to benchmark against Paulatto et al. (2012).	119
6.1	Parameters used to produce figure 5.21.	164

Chapter 1

Introduction

1.1 Motivation

Characterising the internal structure and processes of volcanic plumbing systems has long been a key issue for geoscience. The intricate processes that occur in the Earth’s interior have been widely studied since the turn of the nineteenth century, when the central importance of igneous petrology became abundantly clear through work by eminent geologists such as Charles Lyell and James Hutton. Following Lyell’s prediction that Earth’s crustal diversity was fundamentally derived from igneous processes, early petrologists studied igneous formations in an attempt to determine the parameters governing the production of the observed variety of compositions (Lyell, 1833). Their early studies of magmatic transport and storage have enhanced our understanding not only of how the Earth’s crust formed but also of Earth’s internal processes and continuous rheological evolution (Middlemost, 1991).

The academic interest in magmatic processes has mainly been driven by a need to understand, predict, and mitigate the hazardous nature of extrusive igneous activity. Studies of volcanic eruptions date back well before Lyell’s time to the Roman Empire and the famous eruption of Vesuvius in 79AD, which led to the destruction of Pompeii and surrounding towns, as documented by Pliny (Sigurdsson et al., 1982). The current and historical fascination with volcanic eruptions can be attributed to their wide-spread social, economic, and environmental impacts which have included, but not been limited to; death, damage to property, long-term climatic changes, and destruction of entire habitats and ecosystems. The substantial threat posed by eruptions has therefore led to a demand for an in-depth and robust understanding of volcanic processes. However, despite significant scientific advances made over the last century, particularly with respect to geophysical techniques and petrological observations, current understanding of melt distribution within the complex architecture of sub-volcanic systems is limited (McNutt, 1996; Sparks, 2003). In particular, the dynamics governing magma intrusion, segregation, and storage in the crust are poorly constrained, thereby hampering prediction and mitigation capabilities (Annen et al., 2008).

Ultimately, for successful forecasts to be made, a quantitative method for eruption prediction and determination of the physical state at active volcanic centres must be developed (Scarpa, 2001; Sparks, 2003). In order to model the dynamics of volcanic systems, accurate estimates of the internal geometry of the plumbing system are required (Paulatto et al., 2012). To date however, attempts at constraining the physical and thermal properties of magma systems have had conflicting results from which no consensus has been able to be drawn (Paulatto et al., 2012; Lees, 2007; Voight et al., 2010;

Foroozan et al., 2010). The highly non-linear and dynamic nature of sub-volcanic systems makes precise forecasting an extremely complex task that relies heavily on a quantitative understanding of the causative mechanical and chemical interactions (Sparks, 2003).

1.2 Aims and objectives

The driving force behind this thesis is to improve our understanding of the thermo-mechanical processes in crustal magma systems by comparing numerical modelling results with synthetic velocity models obtained using full waveform inversion to investigate melt distribution in the shallow crust beneath active volcanoes. In addition, this thesis aims to place better physical constraints on crustal melt fraction, geometry, and interconnectivity with the long-term goal of establishing the foundations of a framework for quantitative eruption prediction.

One of the aims of this thesis is to provide a method for converting the results of melt distribution and temperature in the shallow crust, provided by the presented thermo-mechanical model, into two-dimensional velocity profiles containing the intricate structure of the volcanic plumbing system predicted from the model. In addition, the impacts of melt fraction and temperature on background seismic velocity are investigated.

Another key objective of the thesis is to determine the extent to which full waveform inversion is capable of resolving the fine-scale velocity structure of the shallow crust at volcanic centres. The enormous physical extent of the problem makes running the seismic inversions incredibly computationally expensive. As a result, the compromise between computation time and recovery is investigated to assess whether it would be feasible to run a full waveform inversion on geophysical data collected at active volcanoes.

1.3 Structure of this thesis

This thesis is split into three major sections detailing the progressive stages of determining the structure of sub-volcanic crust. Relevant literature is reviewed for each individual section, followed by a detailed discussion of the methods used and results obtained. The first section (chapter 2) describes the model used to determine the spatio-temporal evolution of melt distribution throughout the studied

regions of the crust. This chapter aims to determine the extent of melt produced in various geological situations based on inputs from case-studies. Benchmarks against previous models are set and then temperatures and melt fractions are calculated in the shallow crust during simulation of repeated sill intrusions. The difference between previous purely thermal models and the model incorporating segregation is shown. The third chapter outlines the model used to convert the temperature and melt fraction data into seismic velocity profiles, taking into account the elastic moduli properties of typical igneous petrologies. These synthetic profiles are created for a variety of geological simulations. Various approaches to reproducing the results from temperature and melt fraction inversions on travel-time tomography data, using a purely thermal model, and the differences obtained by including melt segregation are discussed in chapter four. The final velocity models are then used in full wave form inversions in chapter five. The aim in the fifth chapter is to investigate whether or not the synthetic seismic data is capable of being inverted to produce geologically sound profiles of volcanic plumbing systems, and the extent to which FWI is able to resolve the fine-scale detail in the models including melt segregation. The chapters build successively on one another, culminating in an assessment of the effect that maximum inversion frequency has on velocity recovery for FWI in sub-volcanic intrusion zones.

Chapter 2

Literature Review

2.1 Thermo-mechanical modelling

In order to provide insight into the dynamics of volcanic systems, a thermo-mechanical model of coupled melt segregation and crustal compaction has been adapted from Solano (2011). The original model was applied by Solano (2011) to deep crustal hot zones (DCHZs) and mobile magma formation in the lower crust. Specifically, it was used to determine the origin of the observed stratification of the crust between an evolved, broadly granitic upper crust and the more primitive, mafic lower crust (Solano, 2011). Buoyancy driven melt segregation through a permeable, deformable pore space was modelled to determine the effects of melt migration on magma formation, storage, and evolution in deep crustal hot zones (Solano et al., 2012).

The original model of Solano et al. (2012) built upon various previous models which were static and purely thermal. Models such as those of Annen and Sparks (2002); Annen et al. (2006); Annen (2009, 2011); Annen et al. (2014) examine only the effect of increasing temperature on melt distribution in the crust and therefore do not include the effects of melt segregation. While these models have greatly enhanced our understanding of the spatio-temporal evolution of melt distribution their static nature means that they neglect a key feature of multi-phase systems. Namely the fact that pressure gradients arise when there exist multiple phases in a system that have varying densities and viscosities, which in turn leads to flow along the gradients (Richter and McKenzie, 1984). Static models provide a useful first-order estimation of melt volumes and distributions in the crust however they are unable to predict how the melt moves and how the distribution evolves through time when the melt migrates (Solano, 2011). In contrast, thermo-mechanical modelling adds an extra layer of complexity to the underlying physics by including the movement of mass through the system (Solano, 2011). Studies of melt segregation have therefore provided a huge insight into the dynamic processes of sub-crustal systems.

While various studies of deep igneous processes prior to the work of Solano et al. (2012) have shown that a wide range of felsic and intermediate magmas could be produced from the same parent stock of mantle-derived basaltic magma, the mechanism for producing the observed compositional stratification is less clear (Bergantz, 1989; Rushmer, 1991; Clarke, 1992; Atherton, 1993; Tepper et al., 1993; Brown, 1994; Petford et al., 2000; Petford and Gallagher, 2001; Annen and Sparks, 2002; Jackson et al., 2003; Chappell et al., 2004; Dufek and Bergantz, 2005; Annen et al., 2006; Annen, 2009, 2011; Solano, 2011; Solano et al., 2012). Solano (2011) determined the conditions under which melt segregates in DCHZs to produce increasingly more evolved compositions at progressively lower temperatures.

In contrast with purely thermal models that do not include the physics of melt segregation, the maximum temperature and the location of highest melt fraction are found to be decoupled due to magma evolution in the DCHZs (Solano, 2011; Solano et al., 2012, 2014). The modelled influxes of mantle-derived basaltic melt produced felsic mobile magmas at the top of the DCHZs at depths ranging from 27-32km, depending on the style of melt emplacement used in the model (Solano, 2011; Solano et al., 2012). This has considerable implications over the entire depth of magmatic plumbing systems as it suggests that magma evolution may occur throughout the crust rather than solely in shallow magma reservoirs, as had previously been postulated (Bowen, 1915a; Bergantz, 1989; Richter and McKenzie, 1984; McKenzie, 1985; Petford and Gallagher, 2001; Annen et al., 2006; Annen, 2009; Solano, 2011; Solano et al., 2012).

This model has now been further developed by Solano et al. (2014) to include the effects of reactive flow on melt distribution. The matrix into which sills are emplaced is allowed to deform through melt-enhanced creep. A pressure gradient is maintained due to the compositional buoyancy of the melt which allows the melt to rise upward through the crust during simulations. The relative motion of melt and crystals allows for continuous chemical differentiation which is modelled using a binary phase diagram (Solano et al., 2014). Understanding the spatial and temporal evolution of magma, not only in DCHZs but also in the shallow crust, is important for improving current constraints on the physical and chemical processes that lead to volcanic eruptions (Daly, 1914; Bowen, 1915a; Sparks, 2003; Hawkesworth et al., 2004; Solano et al., 2012). This code has been modified further for the simulations shown in this thesis to allow multiple sill intrusion episodes to be modelled. In addition, the model has been adapted and applied to the shallow crust in order to facilitate tracking of the process of melt segregation beneath volcanic centres. The adapted thermo-mechanical model has been used to examine the influence of melt migration on shallow crustal systems and the evolution of magma reservoirs through time. In addition, the method for enthalpy calculation throughout the modelling process has been developed to allow for sills with varying crystal fractions to be intruded in the crust. As a result of these changes, the model is better able to simulate conditions for various intrusion episodes at volcanic centres as well as for varying degrees of melting, thereby facilitating benchmarking tests against various purely thermal models.

The thermomechanical model utilises repetitive sill emplacement in the shallow crust to simulate high temperature, fully molten magma influxes from a deeper melt source. Thermal evolution of the crust following sill intrusions has been shown to be dominated by conduction, despite the fact that magma is able to convect within the sills while the interconnected melt volume fraction is high enough (Brandeis and Marsh, 1989; Marsh, 1989; Bergantz and Dawes, 1994; Jackson et al., 2003). While

convection within intruded sills has been shown to reduce the overall temperature on a shorter time scale, the degree of convection is not enough to significantly affect the results (Annen et al., 2014). Thermal relaxation in between sill emplacements results in melt only being present intermittently until the background temperature has been perturbed far enough from the initial geotherm to sustain melt production, and solidus temperatures have been exceeded (Annen et al., 2006; Annen, 2009; Solano et al., 2012). The numerical description of heat flow in the crust is combined with quantitative modelling of melt segregation processes which determine the extent of melt migration away from the site of initial sill intrusion (Jackson et al., 2003, 2005; Solano et al., 2012).

2.2 Calculating elastic moduli

In order to calculate the seismic velocity profile in a domain where vertical and lateral variations are present in both temperature and melt fraction, the relative contributions to the velocity anomaly must be dealt with separately (Paulatto et al., 2012). In this case, the effect of temperature on the background velocity was dealt with first by assuming that melt fraction was zero and that the velocity anomaly was caused solely by the perturbation to the geotherm (Paulatto et al., 2012). An expression for seismic velocity based on temperature was taken from Karato (1993), which includes effects on velocity from anharmonicity and anelasticity. Karato (1993) showed that for a compositionally homogeneous medium the main source for lateral seismic velocity anomalies derived from lateral variations in temperature. Velocity, density, and temperature have been shown to be proportional, with anelastic and viscoelastic effects on the temperature dependence of seismic wave speeds playing a key role in the crust (Karato and Spetzler, 1990; Karato, 1993). Once the effects of elevated temperatures have been determined, it is possible to determine the additional effect on the seismic velocity profile produced by the presence of melt in the domain.

Estimating the elastic constants in modelled sub-volcanic systems is the first step in converting predictions of melt fractions to give a seismic wave speed anomaly. For the experimental case of a single, homogeneous crystal, the relevant physical constants pertaining to seismic velocity are easy to determine experimentally (Simmons and Wang, 1971; Berryman, 1995). However, in the case of heterogeneous composites, the computation of elastic constants becomes a lot more complicated (Berryman and Berge, 1996). The Voigt-Reuss-Hill approximation is one of a number of calculations which is able to estimate the isotropic polycrystalline elastic moduli of a heterogeneous composite using the anisotropic single-crystal elastic properties (Chung and Buessem, 1967; Berryman, 1995).

The V-R-H approximation is an averaging scheme which takes three component factors (the Voigt average, the Reuss average, and the Hill average), thereby providing upper and lower bounds on the elastic moduli as well as an average value. The Voigt approximation assumes uniform strain in the polycrystalline aggregate while the Reuss approximation assumes uniform stress in the polycrystalline aggregate, thereby giving the upper and lower bounds respectively to the values for bulk and shear elastic moduli (Sun et al., 2004). The Voigt and Reuss bounds for a polycrystalline medium can be used to determine the Hill Average, calculated by taking a simple average of the two values.

It was shown by Hashin (1960) that it is possible to derive more rigorous bounds on the upper and lower estimates for effective elastic moduli of composite materials than the VRH average Hashin and Shtrikman (1961a,b, 1962, 1963). Hashin's approach assumes a uniform volume concentration of particles for a randomly heterogeneous material, effectively producing a quasi-homogeneous material whose effective elastic moduli can be determined through integration rather than simple averaging (Hashin, 1960).

In order to determine the elastic properties through integration, the relative compositional proportions and constituent moduli must first be known (Hashin, 1960; Hashin and Shtrikman, 1961a; Berryman, 1995). For the purposes of this study, where the initial input into the model includes the liquidus temperature, solidus temperature, enthalpies, and broad composition, and the output includes melt fraction calculation, it is possible therefore to determine the upper and lower Hashin-Shtrikman bounds for the effective elastic moduli. While it is theoretically possible to derive more precise estimates for the composite elastic properties, rather than relying on upper and lower bounds, this would require an understanding of the internal stress field and the phase geometry, which in most cases are unknown and not easily determined on the pore scale (Hashin and Shtrikman, 1963; Hill, 1963). The Hashin-Shtrikman bounds therefore provide the most rigorous upper and lower estimates to date for the effective elastic moduli of randomly oriented crystal aggregates, falling within the Voigt and Reuss upper and lower bounds (Watt and Peselnick, 1980; Berryman and Berge, 1996).

The Hill average, which lies between the Hashin-Shtrikman bounds, can be used as a simple estimation for the elastic moduli values in calculations for cases where the bounds are close (Hill, 1952; Hashin, 1960; Berryman and Berge, 1996; Sun et al., 2004). While this gives a good approximation to the bulk and shear moduli, it is possible to improve on the Hill average using the iterative self-consistent approach described by Berryman (2005). Using various assumptions on melt and matrix geometry, it is possible to rapidly converge on a definite and unique solution for both the bulk and shear moduli from the Hashin-Shtrikman bounds using the iterative approach of Berryman (2005).

The inherent benefit of obtaining unique elastic moduli values lies in the ability to convert them to seismic wave speeds and thereby produce a synthetic velocity model for use in tomographic and full waveform inversions (Berryman, 1990). Developing a numerical method for determining the elastic moduli was therefore key in facilitating the final objective of this thesis in calculating synthetic seismic data that was capable of being inverted to produce profiles of sub-volcanic structure. As such, an iterative solver was produced for this thesis which used the melt volume fraction results from the thermo-mechanical model, as well as the other rheological parameters, to solve a pair of coupled equations for the bulk and shear moduli (Berryman, 1980a, 2005; Paulatto et al., 2012). The medium is assumed to consist of two phases - one solid phase, and one melt phase, which are effectively interchangeable within a homogeneous composite (Paulatto et al., 2012). Application of the self-consistent approach of Berryman (2005) allowed for the velocity anomaly produced by the presence of melt to be compounded with that produced by elevated temperatures in the modelled domain.

2.3 Seismic inversion

The final result consists of a high-resolution two-dimensional velocity profile of the modelled sub-volcanic system for both the purely thermal case and the case where the physics of melt segregation is included. The velocity anomalies provide a comparison to previous travel-time tomography inversions at Montserrat carried out by Paulatto et al. (2012) and Annen et al. (2014). In both of these previous studies the seismic velocities calculated from the two way travel times have been used to calculate inverse estimates of temperatures and melt fractions based on predictions from a purely thermal model of the crust beneath the Soufrière Hills Volcano in Montserrat. This specific case-study which compares the results with and without mass transport highlights the importance of including melt segregation in the estimation of the spatio-temporal distribution of melt in the crust. While the thermal model is capable of explaining the observed seismic anomaly, the results obtained by inverting output of the thermo-mechanical model are markedly different. When both the thermal and segregating models are allowed to run for the same length of time with identical sill emplacement rates, the speed at which melt accumulates in the segregating model results in the creation of a mobile magma significantly faster than in the purely thermal case. When segregation and reactionary flow are considered, along with the use of a binary phase diagram to track compositional changes, the spatial and temporal evolution of melt distribution is shown to be significantly different. The melt fraction signatures observed using travel-time tomography and a purely thermal model at Montserrat can be explained with the

segregating model by using either much lower emplacement rates, shorter timescales of emplacement, or long periods of cooling after emplacement.

The aim of this thesis is to produce a comparison between modelled and seismic data to investigate the distribution of melt fractions in the shallow crust beneath active volcanoes. The calculated timeframe over which the melt fractions accumulate via coupled segregation and compaction greatly enhances our understanding of melt residence times in sub-volcanic systems. There is seen to be a significant difference in the volume of melt produced between the simulations with and without active melt segregation over the same period of time. The speed at which melt accumulates when reactive flow and melt segregation are accounted for in the model suggests that the time-frame over which magma is able to become mobile is much shorter than has previously been predicted for the same rate of intrusion in the shallow crust. Results of melt fraction distribution in the shallow crust from the thermo-mechanical model are matched with those using only the thermal model at much higher rates of emplacement and over longer time scales. The reduction in both emplacement rate and timescale required to form a pre-determined volume of melt, and therefore the respective calculated velocity anomaly, when using melt segregation rather than a purely thermal model is one of the key findings of this work.

The results obtained provide a high-resolution model of sub-volcanic temperatures and melt fractions in the upper crust. One of the key objectives of this thesis is to use these predictions of melt distribution to construct a p-wave velocity model and investigate whether the fine-scale details in this model can be recovered using full waveform inversion (FWI). If successful, this demonstrated that we can apply FWI to obtain high-resolution images of volcanic plumbing systems, which is not currently possible using traditional travel-time tomography (Lees, 2007; Virieux and Operto, 2009).

Seismic surveys are essentially a means of mapping the structure of Earth's subsurface by sending down waves of seismic sound energy which are reflected and refracted back to the surface of the Earth (Sirgue et al., 2010b). The seismic waves carry information about the internal physical structure of the Earth to the surface, where the data gathered can be processed to provide information on subsurface velocity and density profiles (Oldham, 1906; Virieux and Operto, 2009). This technique has been used since the birth of modern seismology in the early 20th century when travel-time information from earthquakes, called tele-seismic data, was used to determine the rheological nature of Earth's interior layers (Oldham, 1906; Gutenberg, 1914; Lehmann, 1936).

Seismology has since provided us with a wealth of information about the compositional and structural nature of the crust. Many of the innovations in seismic techniques have been developed by the petroleum industry, where three-dimensional imaging of potential oil fields has reduced costs and improved the efficiency of exploration operations (McQuillin et al., 1984; Haas and Dubrule, 1994). Historically, the majority of detailed seismic acquisition surveys have been in regions with high economic potential for the commercial petroleum industry (McQuillin et al., 1984; Morgan et al., 2013). As such, there exist relatively few high-resolution seismic surveys in active volcanic regions, which generally hold little interest with respect to the potential for commercial hydrocarbon exploitation (Staples et al., 1997).

Seismic imaging beneath igneous rocks is extremely complicated due to the intrinsically multi-component nature of igneous geological systems (Chironi et al., 2006; Lees, 2007; Paulatto et al., 2012). Passive and active seismic tomography have been used to delineate broad regions beneath active centres which exhibit low seismic velocities and are generally interpreted as regions containing relatively high melt fraction (Paulatto et al., 2010; Annen et al., 2014; Voight et al., 2014). However, data noise and low spatial resolution lead to poor imaging with few identifying features (Lees, 2007; Christeson et al., 2008). This is particularly true in the shallow crust, where high-resolution images beneath volcanic centres are extremely rare (Staples et al., 1997; Brandsdóttir et al., 1997; Christeson et al., 2008; Paulatto et al., 2012). Passive seismic surveys are hindered by the inhomogeneous nature of sub-volcanic earthquake distributions, the heterogeneous nature of volcanoes, and low seismic frequencies used for constructing velocity models (Voight et al., 2010).

While active seismic tomography using marine air-gun sources is well suited to island-arc imaging using towed streamers, the computational and financial costs involved means that the number of dense seismic datasets are severely limited (Voight et al., 2010; Paulatto et al., 2012). In addition, seismic travel-time tomography is unable to resolve fine-scale heterogeneities in sub-volcanic crustal structures (Hansen et al., 1999; Paulatto et al., 2010; Shalev et al., 2010). The scale of crustal irregularities can range over several orders of magnitude, from centimetre-scale brecciation to plutons many kilometres across. Travel-time tomographic inversions are only capable of detecting heterogeneities on the order of several hundred metres, which means that diffuse regions of low melt-fraction magma and small scale structures often cannot be identified (Hansen et al., 1999; Lees, 2007).

Full-waveform inversion (FWI) is an advanced data-fitting method which is able to recover high-resolution, high-fidelity seismic velocity models (Virieux and Operto, 2009; Warner et al., 2013). The main advantage of FWI when compared to travel-time tomography is that it has the potential to

resolve structures in the crust on the order of half the seismic wavelength (Virieux and Operto, 2009). In comparison, traditional travel-time tomography approaches are limited in resolution to a Fresnel width, which is on the order of the square root of the product of the ray path length and seismic wavelength (Williamson, 1991). Studies have shown that FWI can be used to determine the nature of small scale velocity structures at large depths (Morgan et al., 2013).

The computationally demanding local optimisation problem, where successive iterations are used in an attempt to minimise the difference between recorded and modelled seismic velocity data, was first described in purely theoretical form by Tarantola (1984). The technique has since been developed for practical use and has subsequently been substantially updated to improve computational efficiency and to include long-offset data (Pratt, 1999; Virieux and Operto, 2009). The introduction of three-dimensional multi-azimuth datasets in various studies has also improved the accuracy of recovered subsurface seismic velocities (Sirgue et al., 2007; Plessix, 2008; Sirgue et al., 2010a; Warner et al., 2013). While the majority of applications to date have been in the oil and gas industry, which has been responsible for the rapid advancement of the technology, FWI has been shown to be capable of providing high-resolution images of sub-sedimentary crystalline crust (Morgan et al., 2013).

Modern applications of FWI use long-offset, low-frequency datasets, with data acquisition from wide-angled seismic surveys (Sirgue et al., 2010a; Vigh et al., 2011, 2013). Theoretically, FWI accounts for the entire wavefield, honouring all of the physics of wave propagation, and is therefore in principle able to recover a subsurface model of any property that affects the recorded seismic wave-field (Operto et al., 2013; Prieux et al., 2013a,b). In practice however, commercial applications of FWI generally use an acoustic approximation to the wave equation and only recover the P-wave velocity model (Virieux and Operto, 2009; Kapoor et al., 2013; Warner et al., 2013).

For the case of synthetic seismic data, where the true velocity model is known prior to carrying out FWI, building a sufficiently accurate starting model is relatively uncomplicated. While experimental field data often requires the use of additional complex procedures to build a starting model, such as stereotomography or Laplace-domain inversions, synthetic datasets only require the true data to be simplified and smoothed to give a realistic initial approximation (Virieux and Operto, 2009). For this particular study however, the thermo-mechanical model predicts only the subsurface temperature, enthalpy, and melt fraction values. As such, prior to a full waveform inversion being implemented, a synthetic velocity profile had to be derived from the modelled subsurface parameters. The calculated velocity profile was then used to explore how the maximum inversion frequency used in FWI affects velocity recovery. This was done by comparing the results after inversions at progressively increasing

frequencies. The maximum inversion frequency is one of the constraining factors on resolution when carrying out FWI. FWI run time scales with model sizes, and with large data-sets such as those that would be expected for sub-volcanic intrusion zones, it is important to explore the potential improvements to the recovered velocity structure provided by high-frequency inversions as they may not be affordable.

2.4 Conclusion

On-going research into the dynamics of sub-volcanic systems would greatly benefit from the ability to use full waveform inversion to investigate the structure of the shallow crust at active volcanic centres. The methods outlined above and explained throughout this thesis provide a framework for predicting melt distributions in the shallow crust and using these predictions to develop high-fidelity, high-resolution seismic inversions at active volcanic centres. While the work in this thesis has been carried out on synthetic seismic velocity profiles, it is shown that the technique can be used on real seismic data. In addition, the investigation into domain scale would benefit future studies as it examines the physical extent of seismic surveys that can realistically be carried out and applied to a full waveform inversion of the sub-volcanic crust.

Chapter 3

Thermo-mechanical Model - Description and Benchmarking

3.1 Background

Magmatic processes have contributed to the nature of Earth's crust since its formation, providing the foundations for Earth's diverse crustal lithologies (Lyell, 1833). As such, the study of igneous processes gives insight not only into Earth's formation 4.5 billion years ago, but also into its ongoing petrological evolution. The early twentieth century saw a marked advancement in theories concerning igneous petrology and the principles of magma production. Building upon previous works by R. A. Daly and A. Harker, petrologist N. L. Bowen theorised that for the case of a fully molten magma chamber, differentiation and evolution of the magma occurred principally through crystallisation and crystal settling (Harker, 1909; Daly, 1914; Bowen, 1915a,b).

Bowen described the life-cycle of magma formation as a continuous chemical and physical process, showing that the formation of mobile magmas with diverse rheological profiles was possible from a single source of mantle derived melt (Bowen, 1915a,b). The mechanism for this evolution was postulated to be fractional crystallisation, where different compositions solidify and fractionate out of the mixture as it cools at progressively lower temperatures (Bowen, 1915b). The crystals were shown experimentally to sink through synthetic mixtures by gravity and to settle at the base of the modelled reservoirs Bowen (1915b). Consequently, this led to the theory of vast, long-lived liquid magma reservoirs that reside in the crust and act as the site of magmatic chemical differentiation - termed magma chambers (Bowen, 1922).

This orthodox view of a molten reservoir of magma is compelling, particularly as it is capable of accounting for the production of a full range of evolved magmatic compositions, as seen in both intrusive and extrusive igneous rocks, from a common basaltic stock (Caricchi and Blundy, 2015b). As a result, the long-standing assumption of the existence of these magma chambers has been perpetuated by results obtained, and methods used, in various chemical and physical models (Huppert and Sparks, 1988b; Petford et al., 2000; Annen et al., 2006; Annen, 2009). Bowen's influence has been used to determine the model domain and style in a wide range of work dedicated to studying magma evolution in the crust, utilising the traditional liquid-dominated magma chamber as an end-point for these models (Huppert and Sparks, 1988b; Petford et al., 2000; Annen et al., 2006; Annen, 2009). However, Bowen's description of magmatic evolution through the separation of multiple distinct phases from a fully liquid reservoir, with fractional crystallisation dictating the magma chamber dynamics, has recently been put into question (Jackson et al., 2005; Solano et al., 2012; Jackson et al., 2018). New evidence has emerged to suggest that the large liquid vat assumption may not be the principal method

through which crustal melts evolve, bringing into question the role of magma chambers in the spatial and temporal evolution of melt composition and distribution.

It has been shown that fractionation resulting in crystal settling is not efficient enough to be the sole mechanism for separating solids and liquids. Particles held in a dense suspension are in fact subject to hindered settling, as set out by Davis and Acrivos (1985). As a result, in Bowen's case of a large magma reservoir, the increasing crystal fraction in the reservoir with time during cooling would produce conditions where it would become increasingly difficult for differentiation and settling of crystals to occur. In the last stages of their evolution the two-phase differential flow required between crystals and melt, to allow magma to evolve by crystal fractionation, would no longer occur (Bachmann and Bergantz, 2004). This poses a problem in that ongoing differentiation would result in large volumes of chemically distinct trapped magma pockets, effectively forming magmatic breccias which are not observed in field samples or using geophysical sub-surface imaging techniques (Glazner and Bartley, 2006). The conglomerate-style intrusive bodies that would most likely form under hindered settling in a magma reservoir are therefore inconsistent with both field and geophysical observations of high silica granites and interleaved mafic-felsic layering in the shallow crust (Cheadle et al., 1987; Bachmann and Bergantz, 2004; Solano, 2011; Lee and Morton, 2015).

In addition to the difficulties incurred with crystal settling, there is mounting evidence that volcanic plumbing systems and the chemical evolution of magma in the crust may not be as simple as Bowen's reaction series model of crystal fractionation suggests. As discussed by Glazner et al. (2004), there is little seismic evidence in the crust for melt fractions above 10%. This suggests that there exist very few large mobile magma bodies, defined by Jackson et al. (2003) as having liquid volume fractions above the Solid Liquid Transition (SLT), the point at which the bulk rheology changes and melt becomes fully interconnected along grain boundaries and is able to become mobile, occurring at melt fraction $>0.4-0.6$ (Jackson et al., 2003; Rosenberg and Handy, 2005; Solano, 2011). Glazner et al. (2004) demonstrated that magma volumes with high melt fractions exhibit heterogeneous layering and further geochronological evidence suggests that they form through incremental accretion as opposed to being emplaced as a single large liquid vat (Annen, 2009, 2011).

Despite the abounding evidence that crystal fractionation does not dominate magma chamber dynamics as postulated by Bowen, various purely thermal models of magmatic systems have been developed where fractionation dictates the modelled spatio-temporal melt evolution and distribution. While the model domains vary according to the study areas, which span a large portion of the crust from Deep-Crustal-Hot-Zones to shallow (<5 km) emplacements, the models all predict the production of

expansive molten bodies following incubation of magma intrusions in the crust at high temperature (Halliday et al., 1989; Petford and Gallagher, 2001; Clemens, 2003; Annen and Sparks, 2002; Annen, 2009). These models require very high one-dimensional emplacement rates ($>10\text{ mpa}$, Annen (2009)) of mantle-derived basaltic melt in order to create bodies of mobile magma similar to Bowen's liquid vat hypothesis through repetitive sill emplacement (Petford and Gallagher, 2001; Annen, 2009, 2011). While geophysical evidence has been found for such high emplacement rates in the crust in the past, they have been shown to be transient and short lived (Hanson and Glazner, 1995; Spera and Bohrsen, 2004). Measured heat fluxes in the shallow crust have been estimated as being due to much lower average long term melt emplacement rates (Huppert and Sparks, 1988b,a; Hanson and Glazner, 1995; Spera and Bohrsen, 2004; Jackson et al., 2005). When coupled with the lack of observed evidence in the field for the large, high melt fraction igneous bodies that would be required to maintain these high liquid volume fractions for extended geological time periods, the argument for the formation of accumulated long-lived liquid magma chambers appears tenuous (Jackson et al., 2005; Solano et al., 2014; Caricchi and Blundy, 2015b; Riel et al., 2016, 2018).

While processes such as magma mixing, dehydration melting of amphibolites, and partial melting of crustal rocks have been shown to be capable of producing highly evolved melts, it has also been shown that these processes are not efficient when discussing large scale igneous intrusions (Glazner, 1994; Chappell and White, 2001). Granitic melts are commonly produced at low degrees of melting from their source rock, typically with melt fractions on the order of 0.1-0.4 due to the low melting temperatures of felsic minerals (Rushmer, 1991; Solano, 2011). As a result, the volume of source rock required to produce large quantities of in situ granitic melts through magma mixing or partial melting would result in large mafic cumulates left behind in the crust, often in excess of two thirds of the parent rock volume (Mahood and Halliday, 1988; Rushmer, 1991; Solano et al., 2012). There is a distinct lack of geophysical evidence for any such cumulates however, and to date there have been no field observations of the required large mafic bodies in studies of exhumed crust (Glazner and Miller, 1997; Glazner and Bartley, 2006; Petford et al., 2000).

This suggests that the production of the broadly granitic upper crust does not occur through simple differentiation of magma mixing in situ but rather begins with a basaltic source emplaced in the lower crust (Jackson et al., 2003; Solano et al., 2012). Buoyancy coupled with the continuous chemical evolution of melt as it travels through, and equilibrates with, its surrounding country rock has been shown to result in stratification of the crust, from a more mafic lower crust to a felsic shallow crust (Annen, 2009; Solano, 2011; Solano et al., 2012). While it was argued by Glazner and Miller (1997) that the absence of cumulates may be due to their negative buoyancy and subsequent sinking through the

crust, this argument lacks observational evidence and has since been retracted in various subsequent works (Glazner et al., 2004; Glazner and Bartley, 2006). Further petrological studies have shown that there exists a textural complexity within the fabric of intrusive igneous bodies that cannot be reconciled with simple fractional-crystallisation (Paterson et al., 2011; Cashman and Blundy, 2013; Caricchi and Blundy, 2015b). Rather it appears as though large igneous bodies are formed over long periods of time that allow for continuous chemical and physical interaction in a highly crystalline mush over a range of temperatures (Solano et al., 2012). This theory is also able to account for the complex geochemical signatures found in exhumed intrusive bodies (Solano et al., 2014; Caricchi and Blundy, 2015b).

Bowen’s classical idea of a large liquid magma chamber therefore does not marry well with geophysical observations or recent modelling. The process of fractional crystallisation, while chemically sound, cannot be invoked to explain the granitic (*sensu lato*) upper crust. In addition, the large volumes of magma produced in numerical models that use Bowen’s approach to form large liquid vats require temperatures to be maintained above the solidus over long geological timescales (Annen and Sparks, 2002; Annen et al., 2006; Annen, 2009). While this may occur transiently during accretion of a large shallow igneous body through multiple sill intrusions, maintaining a simultaneously high melt volume and high temperature body over long timescales would require very fast one-dimensional intrusion rates of $>0.5\text{m/ka}$ to be sustained (Annen and Sparks, 2002; Annen, 2011; Paulatto et al., 2012). Not only would this result in a large heat signature in the shallow crust, measurable as a thermal anomaly on the surface, but also in geodynamic uplift, for which there is currently no geophysical evidence (Annen and Sparks, 2002; Spera and Bohrsen, 2004; Chang et al., 2007). Another difficulty with the traditional liquid-dominated, long-lived magma chamber paradigm is that large liquid volumes, modelled in various cases to be over 10km in diameter, simply would not be capable of supporting the over-lying crust on modelled geological timescales (Annen, 2009; Paulatto et al., 2012; Cashman et al., 2017).

While seismic and magnetotelluric data have identified numerous geophysical anomalies in the crust on the scale of modelled magma chambers, their signatures are not consistent with large liquid reservoirs but rather partially molten bodies with low melt fractions (Ward et al., 2014; Comeau et al., 2015). These intrusive complexes have seismic and geodetic signatures that suggest melt fractions below the solid-liquid transition (Cooper and Kent, 2014; Ward et al., 2014). Various studies have concluded from geochronological and geochemical data that high melt fraction reservoirs are simply a transitory phase in the life-cycle of volcanic plumbing systems, suggesting that differentiation is not the primary

driver of magma chamber dynamics (Cooper and Kent, 2014; Wotzlaw et al., 2014; Caricchi and Blundy, 2015b).

Theoretically, mafic magmas with low viscosities are capable of rising buoyantly through dikes at velocities as high as 0.7 ms^{-1} , thus being capable of producing a large molten magma chamber on timescales of 10^1 - 10^4 years. However, the emplaced volumes would have to be displacing highly crystalline, viscous crustal material at the same rate (Clemens and Mawer, 1992; Rutherford and Hill, 1993; Petford et al., 1996; Coleman et al., 2004). Displacement of this magnitude would result not only in a geodetic signature at the surface but also in substantial tectonic uplift for which there is no geophysical evidence to date (Spera and Bohrson, 2004; Chang et al., 2007).

Evidence from multiple study areas including the Adamello Batholith in Italy, and both the Tuolumne Suite and Mount Stuart Batholith in the USA, suggests that the ages of individual zircon crystals span many millions of years (Coleman et al., 2004; Matzel et al., 2006; Schoene et al., 2012). Despite this, the physical extents of these intrusive igneous study areas would require timescales of less than 1Ma from the final emplacement to cool to a temperature below the solidus (Glazner et al., 2004). While there is still much that is unknown about zircon crystal formation, this evidence appears to make producing and sustaining a large magma chamber emplaced in one single batch geochronologically impossible.

Recent models advocate the idea of a crystalline mush beneath volcanoes, defined by Caricchi and Blundy (2015b) as having a melt volume fraction $<40\%$ which accumulates over time through repetitive cycles of molten magma intrusion and crystallisation (Annen, 2009). This alternate model is based on evidence from the field and recent studies which modelled the phase change and transport processes occurring in multi-component crustal matrices using repetitive sill intrusions (Jackson et al., 2003; Glazner et al., 2004; Jackson et al., 2005; Annen, 2009; Solano, 2011; Solano et al., 2012). It is this idea of crystalline 'mushmatism' - rather than liquid dominated magmatism - occurring throughout the crust that is behind the thermo-mechanical modelling presented in this thesis.

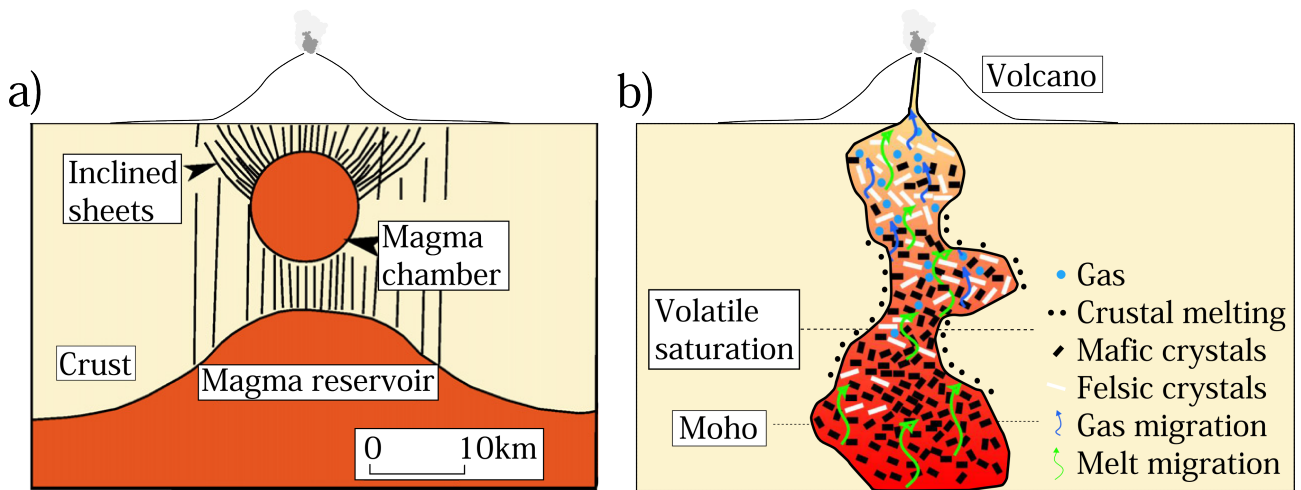


Figure 3.1: Adapted from Jackson et al. (2018). a) depicts the traditional concept of a sub-volcanic magma chamber as a liquid reservoir in the shallow crust. b) depicts a mush column with high crystal fraction with melt segregation occurring between the grain edges of the crystals.

3.2 Early thermal modelling

Early studies of the spatial and temporal evolution of crustal melt employed a single magma emplacement as being responsible for the creation of Bowen's large liquid vat model (Huppert and Sparks, 1988b). This led to the assumption of rapid ascent of fully molten magma through the crust from the site of melting to the site of emplacement, which in the case of shallow crustal emplacement would be a distance on the order of many tens of kilometers (Marsh, 1978). These models assumed that magma accumulation in the crust occurred over very short timescales in order to produce Bowen's picture of a fully molten magma reservoir (Marsh, 1978). This resulted in the formulation of the idea by Marsh (1981), that the total lifetime of a crustal residual melt of any particular composition must be inversely proportional to the rate at which the melt cooled. The melt compositions within these rapidly emplaced magma chambers were predicted to be primarily dependent on the temperature at any given time (Marsh, 1981). As a result, melt fraction and temperature within the modelled magma chambers were fully coupled, with the solidus temperature of the melt controlling the point at which melt fraction reduced to zero, as described by Annen (2009).

Utilising Bowen's logic of fractional crystallisation, the composition of the remaining melt in the modelled magma chambers became increasingly felsic during cooling (depicted by Bowen's series of fractional crystallisation in Figure 3.2) as temperatures relaxed back to the geotherm after an influx of melt (Annen, 2009, 2011).

Subsequent thermal modelling used Bowen's theory of fractional crystallisation within these shallow reservoirs to account for the production of highly silicic large intrusive igneous bodies in the shallow crust (Bowen, 1945; Glazner et al., 2004; Sisson et al., 2005). However, the large scale compositional zoning that results from invoking fractional crystallisation as the dominant mechanism for melt evolution in these models is rarely observed in exhumed field specimens or through geophysical observations (Halliday et al., 1980; Coleman et al., 2004; Annen et al., 2006). Further field evidence of sheeting at margins of large igneous bodies, coupled with isotope geochemistry data and observed hyper-solidus deformation, indicates that intrusive bodies assemble through repeated intrusions over geologically significant timescales, such as at the Tuolumne Intrusive Suite in California and the Ivrea-Verbano Zone in Italy (Lu et al., 1997; Glazner et al., 2004; Solano et al., 2012).

These key indicators of incremental growth of intrusive igneous bodies bring in to question the validity of Bowen's large liquid reservoir theory (Bachmann and Bergantz, 2008; Cashman et al., 2017). In addition, when coupled with geochronological observations of a trend for regularly diminishing ages toward the centre of both individual plutons and their respective igneous suites, the evidence heavily supports emplacement via repeated discrete intrusions as opposed to a single large body (Annen, 2009; Coleman et al., 2004; Glazner et al., 2004). The chemical and physical evolution of a magma body emplaced via successive sills is fundamentally different to that of a similar volume of magma emplaced instantaneously (Coleman et al., 1995, 2004; Annen, 2011). As such, the spatial and temporal evolution of melt cannot simply occur as a result of fractional crystallisation in a liquid vat. Rather, it must reflect the processes that occur during the periodic melt influxes and cooling stages that take place when intrusive igneous bodies are successively emplaced in the crust.

Extensive thermal modelling work has been carried out utilising the method of incremental accretion of sills in the shallow crust (Huppert and Sparks, 1988b; Petford et al., 2000; Annen and Sparks, 2002; Annen et al., 2006; Annen, 2009, 2011; Paulatto et al., 2012). These models investigate magma system dynamics in a two-dimensional, axis-symmetric system which produces a pseudo-3D estimation of melt distribution during thermal evolution (Annen, 2009; Paulatto et al., 2012). Calculations for the transfer of heat energy in previous models have generally been conducted using explicit finite difference algorithms, with many employing symmetry conditions at the central axis as described in Figure 3.3 (Annen, 2009).

The final plutons in the majority of recent thermal models grow via accretion of tabular bodies which are circular in map view, as shown in figure 3.3 (Annen, 2009). The geometry of the individual

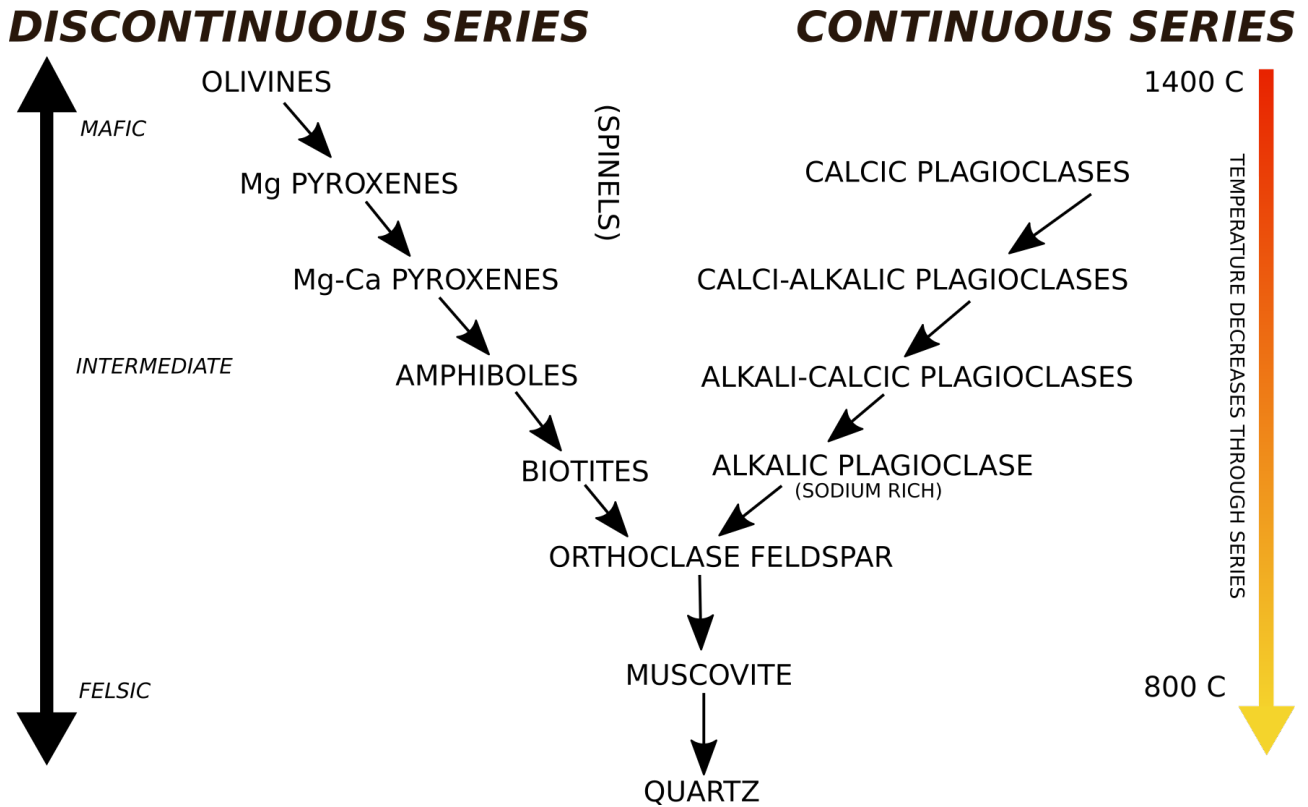


Figure 3.2: The Bowen Series, showing the evolution of melt content from mafic to felsic during cooling. Adapted from Bowen (1922).

emplacements are based on field observations and subsequent mechanical modelling of intrusively emplaced granitic bodies (Vigneresse, 1995; Cruden, 1998). Field and geophysical observations of well defined vertical outer pluton edges and seismic evidence for their low aspect ratios enable the use of the simple model geometries in the majority of model domains (McCaffrey and Petford, 1997; Cruden, 1998). These simplifications improve computational efficiency which is paramount when dealing with large-scale problems such as those defined by Annen (2009), whose numerical simulation emplaces individual sills up to 10 kilometres in radius and 200 metres thick.

Justification for the accretion dynamics commonly used in this work and by various previous numerical simulations, involving stacking multiple sills to form a pluton (Figure 3.3), comes from the work of Menand (2008), who studied the physics of horizontal sill emplacement. Menand (2008) showed that the rigidity contrast produced by a sill emplaced in the crust results in anisotropic rigidity conditions which support the successive emplacement of further sills, capable of accreting to form a large intrusive

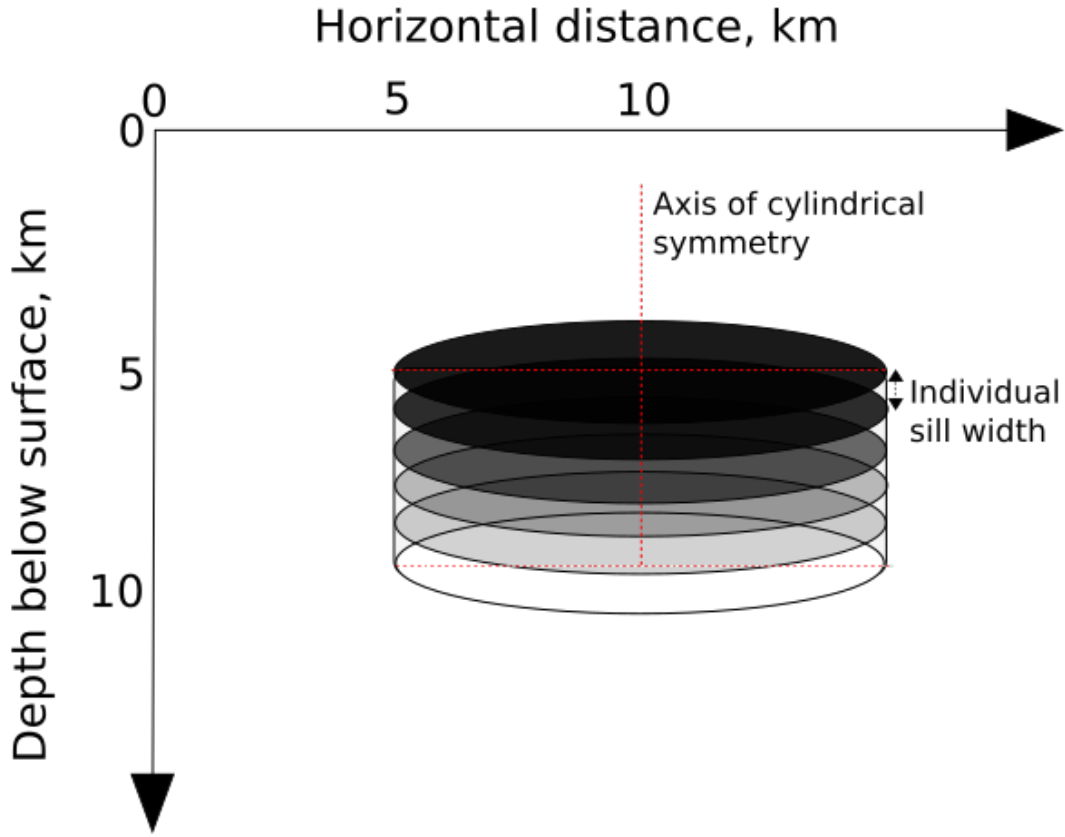


Figure 3.3: Adapted from Annen (2009), this shows the model domain and sill emplacement style of previous purely thermal models. The centre of the domain uses an axis of symmetry to produce a pseudo-3D domain from the 2D calculations of heat transfer. Drawing is not to scale.

body. The subsequent emplacements occur along the rigidity contrasts either below, above, or in the middle of the previous sill. This produces the vertical expansion of igneous bodies which has been adopted in attempts to model magma chamber formation via repetitive sill emplacements (Menand, 2008; Annen, 2009). The model used in this thesis makes space for in-coming sills via downward displacement of the model domain from the point of emplacement. This method is common practice for mechanical models of various intrusion styles and is well aligned with geochronological evidence of field measurements for the ages of strata at exhumed volcanic centres (Paterson et al., 1996; Cruden, 1998).

The majority of early work which was undertaken to study the sub-surface dynamics at active volcanoes used purely thermal models which were a first-order approximation of the processes involved in

these complex systems. Heat transfer occurs in these models purely by conduction, with thermal conductivity remaining constant throughout the model domain (Annen, 2009). While it has been shown that it is possible for convection to occur within the liquid portion of the intruding sills, this is greatly hampered as soon as crystallisation begins due to cooling (Jackson et al., 2003). Magma convection is therefore limited to volumes whose melt fraction exceeds the solid-liquid-transition value, thereby severely restricting the volume through which convection is able to occur and rendering it incapable of changing the order of magnitude of energy transfer in the system (Annen et al., 2008). In addition, convective transport of heat away from the sills through gas sparging into the country rock has been shown to be negligible, thereby justifying the use of conduction as the only form of heat transport (Bergantz and Dawes, 1994; Jackson et al., 2003; Bachmann and Bergantz, 2006).

Purely thermal models are able to sustain magma volumes with high melt fractions when the temperature of the developing pluton is maintained above the solidus temperature. As the system cools following the influx of hot molten material, the temperature profile relaxes back to the initial geotherm. In order to produce and sustain a mobile magma, thermal models therefore require high rates of magma influx. The first sills, which are emplaced into a relatively cold and brittle crust, cool rapidly and fully solidify. Each successive sill then incubates the emplacement zone as latent heat is transferred to the surrounding crust. This reduces the temperature gradient at the point of contact between the emplaced sill material and the country rock. When the temperature exceeds that corresponding to a melt fraction above the solid-liquid-transition in between emplacements, the system forms a crystal mush (Annen, 2009; Solano et al., 2012). The time between the first sill being emplaced and the formation of a mobile magma is termed the incubation period (Annen, 2009).

When a melt volume fraction of 60% has been surpassed between emplacements melt is able to become fully interconnected and form a mobile magma body (Solano et al., 2012). It is at this point, when the total melt volume that exceeds the point of mobile magma formation is greater than the volume of a single sill, that purely thermal models define the creation of a magma chamber (Annen, 2009). As temperature is the driving factor in melt production and melt fraction maintenance, models which only take thermal diffusivity into account find that the point in the magma chamber of highest melt volume fraction occurs at the point of highest temperature. This can be seen in the work of Annen (2009, 2011), where the large, long-lived magma chambers produced by numerical simulation of thermal evolution are at temperatures far exceeding the country rock solidus.

For the numerical simulation run by Annen (2009) with 200 metre thick tonalitic sills, emplaced at their liquidus temperature of 990°C into a country rock of the same composition and a solidus

temperature of 760°C, the temperature at which a magma chamber is sustained was found to be 875°C. Annen (2009) uses under-accretion of sills at an initial emplacement depth of 5km, resulting in the formation of a sustained mobile magma after 25,000 years. The one-dimensional emplacement rates required in order to produce a large magma chamber using this method have been shown in various thermal studies to exceed $3 \times 10^{-2} \text{ myr}^{-1}$ (Hanson and Glazner, 1995; Yoshinobu et al., 1998; Annen et al., 2008; Annen, 2009). For the case of one-dimensional accretion rates $< 3 \times 10^{-2} \text{ myr}^{-1}$ in simulations that only take in to account thermal diffusivity during the spatial and temporal evolution of melt, the required time scale over which a mobile magma forms exceeds 100,000 years (Petford et al., 2000).

For low emplacement rates mobile magmas only form when the emplacement style is intrusion via under-accretion (Solano, 2011; Solano et al., 2012). As the emplacement depth increases with each new sill, the intrusions are emplaced into successively hotter crust due to the linearly increasing geotherm. The increasing background temperature consequently decreases the temperature gradient between the incoming sill and the surrounding country rock, thereby leading to sustained melting and the formation of a mobile magma. Due to the nature of thermal models, high melt volume fractions would not be sustainable if the mobile magma were to migrate upward into the cooler shallow crust. If the melt migrated to shallower depths the surrounding rock would be below the critical temperature for sustaining a mobile magma. The crystal fraction would therefore increase due to cooling, and the magma would stall.

This is clearly a limiting factor in the ability of thermal models to simulate the production of eruptible volumes of melt. The crust does not usually exist in a partially molten state but thermal models require large quantities of heat to be supplied via intrusion of hot material for crustal melting to occur (Solano et al., 2012). While large magma chambers can therefore be modelled thermally using high emplacement rates, there is little geophysical evidence for continuous high melt fluxes in the crust over long timescales (Hanson and Glazner, 1995). In addition, measured heat fluxes above active volcanic centres are much smaller in magnitude than those required by the numerical simulations to form mobile magmas (Huppert and Sparks, 1988b,a; Spera and Bohrsen, 2004). As a first approximation, thermal models provide a useful estimate to the processes involved in melt evolution however, they are not able to fully describe the dynamics of mass transfer involved during repeated heating and cooling of the system.

The key issue with thermal models is that they do not account for mass exchange during melt evolution. More specifically, they do not take in to account melt migration through buoyancy or compaction of

the surrounding matrix and so only partially describe the physical and chemical processes involved in the spatio-temporal evolution of melt distribution in the crust (Jackson et al., 2003; Solano, 2011). The process of melt segregation was incorporated by Solano et al. (2012) and coupled with melt compaction to produce a more holistic thermo-mechanical model.

3.3 Melt segregation and reactive flow

Melt segregation has been incorporated in mechanical models of multi-phase systems since the middle of the twentieth century when melt dynamics from metallurgical studies were applied to geological systems (Behr and Schroeder, 1942; Sleep, 1974). Melt segregation is defined as the buoyant flow of partial melt fractions relative to a solid matrix to the point where the partial melt volume accumulates significantly and forms a mobile magma, thus allowing it to migrate away from its restite and the initial region of melt production (Wickham, 1987; Brown, 1994; Sawyer, 1996).

In the case of crustal granitic melt production, the interconnected solid matrix through which the melt flows must be permeable in order for segregation to occur (Jackson et al., 2003). It has been shown both experimentally and theoretically that the source rock matrix may be permeable at porosities as low as 4% (Bargen and Waff, 1986; Wolf and Wyllie, 1991; Wark and Watson, 1998; Cheadle et al., 2004). Given that the degree of melting necessary to produce highly felsic melt fractions is relatively small (10-40%), this suggests that large, felsic bodies of mobile magma do not form in situ, but rather that melt segregation through the low porosity, but permeable, source rocks provides a mechanism for granitic melt to accumulate (Solano, 2011).

For segregation to be possible, a pressure gradient must exist to drive the flow of melt relative to the surrounding matrix. The natural buoyancy of melt relative to its solid counterpart with the same chemical composition provides the pressure gradient required for flow (Richter and McKenzie, 1984; Ingham and Pop, 1998). In order for melt to accumulate the crust must deform to accommodate it. Evidence for matrix deformation via melt-enhanced diffusional creep can be simulated both in numerical modelling and observed in cross sections of exhumed crust (Richter and McKenzie, 1984; Jackson et al., 2018). It is the coupled segregation and compaction, described in figure 3.4, and the addition of reactive flow which sets the thermomechanical modelling used in this thesis apart from previous, heat-driven modelling (Solano et al., 2012; Jackson et al., 2018).

The study by Solano et al. (2012) built upon previous thermal models of melt generation in deep crustal hot zones (DCHZs) as well as models of matrix compaction during buoyancy-driven upward flow of melt in multi-phase systems. By linking the thermal and mechanical systems in the context of DCHZs Solano et al. (2012) were able to include the migration of melt away from the initial emplacement zone and thereby study the evolution of melt distribution with time.

Solano et al. (2012) used the principles laid out by Richter and McKenzie (1984) to model the physics involved in melt segregation. Figure 3.4, adapted from Richter and McKenzie (1984), depicts the formation of high melt fraction layers in a column of initially uniform, low fluid content. The inherent buoyancy of the melt allows it to move upward through the pore spaces and along grain boundaries whilst the matrix simultaneously deforms and compacts. The high temperature of the pre-existing fluid causes melting to occur along the grain boundaries, resulting in increasing melt fractions with time (figure 3.4 b). This eventually results in three distinct regimes as depicted in figure 3.4 c. The base of the column exhibits densely packed grains with a compacting boundary layer, followed by a non-compacting regime where reactive flow of melt occurs, and a top boundary layer where pure melt accumulates (Richter and McKenzie, 1984). The total amount of compaction is small, with previous models of coupled segregation and compaction showing on average less than a 10% reduction in thickness of a compacting column (Richter and McKenzie, 1984; Solano, 2011; Solano et al., 2012).

The compaction method used in the thermomechanical model of Solano et al. (2012) is a modification of the McKenzie formulation, which assumes that matrix compaction occurs via melt-enhanced diffusional creep (McKenzie, 1984, 1985). This assumption is consistent with the idea that mush reservoirs exist at or above the solidus temperature. Strain rates found for diffusional creep of highly crystalline mushes are low ($<<10^{-15}\text{s}^{-1}$) and result in a Newtonian style rheology for both the melt and the crystal-rich mush mixture (Richter and McKenzie, 1984; Jackson et al., 2018).

One aspect of modelling melt segregation is accounting for the reactive flow of melt, which is in contact with the matrix through which it flows, allowing efficient exchange of both heat and mass through solid and liquid phases present in the mush reservoir (Jackson et al., 2018). The melt and matrix are in constant thermal and chemical equilibrium, meaning that the chemical composition of the melt evolves during melt segregation (Solano et al., 2012, 2014).

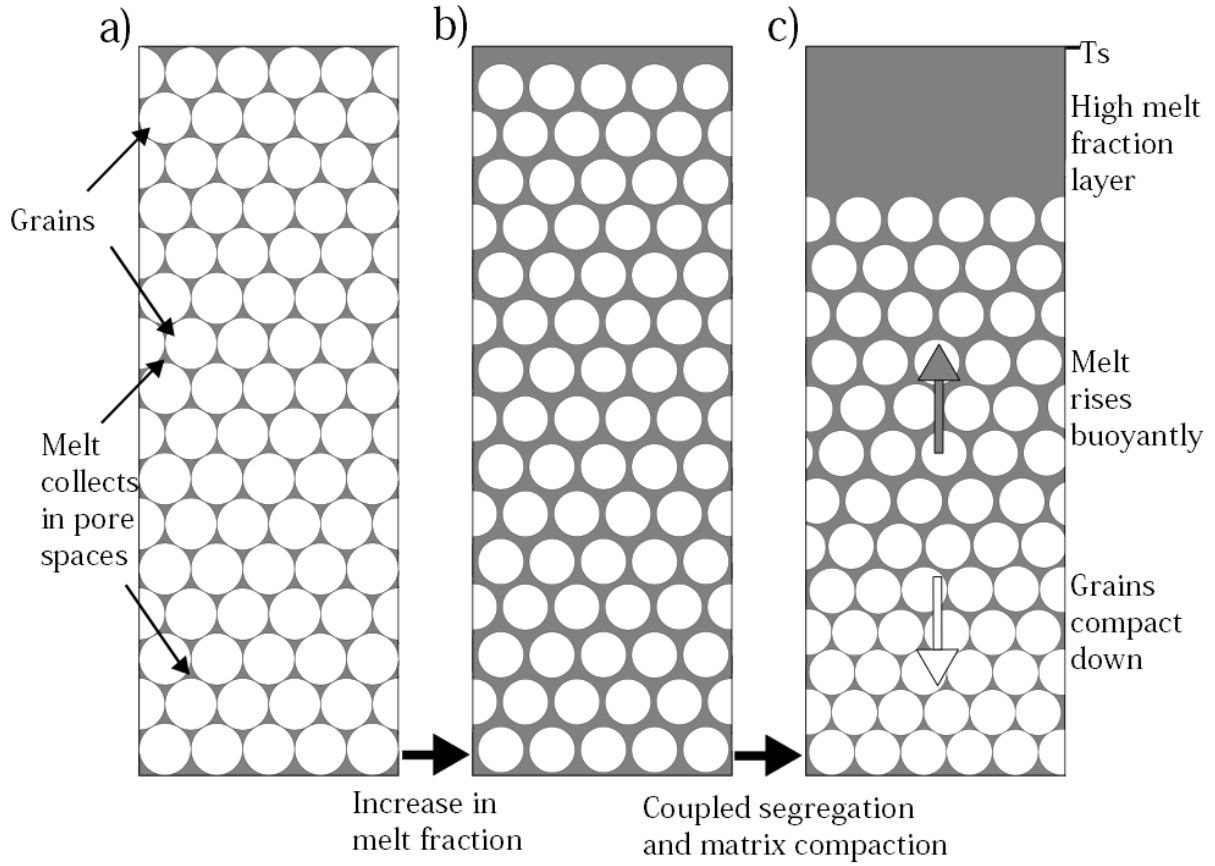


Figure 3.4: Adapted from Richter and McKenzie (1984). a) At low melt volume fractions, below the SLT, grains remain interconnected and melt accumulates in the pore spaces between the matrix grains. b) As melting occurs and melt volume fraction increases the melt becomes interconnected along the grain boundaries. c) Buoyancy driven melt segregation occurs simultaneously with downward compaction of the solid matrix, producing a high melt fraction layer at the top of the column as the melt accumulates. The top boundary marks the point where the column is capped at the solidus temperature. Drawing is not to scale.

The model first developed by Solano (2011) employed the enthalpy method to describe energy transport and the thermodynamics involved in melting. This sets the condition of thermodynamic equilibrium across the entire modelled domain (Katz, 2008). Constant release of latent heat during melting is assumed in the enthalpy method with the thermodynamic properties of the fluid and solid remaining constant and the same (Solano, 2011).

The thermomechanical model originally developed by Solano (2011) included chemical component transport to address the change in bulk melt composition through time during segregation. Whilst being a generalised over-simplification of the dynamic chemical processes occurring in mush systems, this addition was a great improvement on early thermal models. By including evolving local bulk compositions in mush reservoir modelling, Solano et al. (2014) were better able to match experimental melting relationships found for common igneous systems (Jackson et al., 2018).

Further improvements to the thermomechanical model have since been made by Jackson et al. (2018) to better understand the effects of chemical mush interactions during reactive flow. Jackson et al. (2018) included the effects of compositionally dependent melt viscosity, matrix density, and melt-matrix density contrast in their solution. While Solano et al. (2012, 2014) used a melting relationship similar to that of Annen et al. (2006), a binary eutectic phase diagram has been utilised in the thermomechanical model adapted by Jackson et al. (2018). The two-component phase diagram models compositional changes in local bulk composition under the assumption of local thermodynamic equilibrium within the mush.

The thermo-mechanical model is currently not set up to include the effects of surface tension, crystallographic defects, and interphase pressure. In addition, stresses caused by magma chamber over-pressure and tectonic stresses have been neglected. Due to the complex nature of including the response to all of these extra stresses, the thermo-mechanical model is consistent with earlier modelling in neglecting them. It is assumed that the pressure gradient which drives buoyant flow dominates the system during melt segregation and accumulation under the Boussinesq approximation, making the current formulation of the model more than capable of describing the shallow volcanic systems being studied (Solano, 2011). Further developments to the model will look to include these additional stresses to determine the extent of their impact on the spatial and temporal evolution of melt distribution in the crust.

3.4 Method

The governing equations for matrix compaction and heat conservation were developed initially by Solano (2011) building on the model of Jackson et al. (2003) to describe the coupled processes of melt segregation and phase change in the system. The transport of heat and mass, including chemical components, was modelled in one dimension. This simplification is possible due to the high aspect ratio nature of sills in the crust. Vertical bi-directional flow of the melt and matrix has been shown to dominate the advection within intrusive igneous bodies (Petford et al., 2000; Menand, 2008). While a 1-D modelling approach is not able to capture the dynamics of non-vertical flow paths during melt segregation which have been shown to occur under mantle conditions. However, this thesis models the shallow crust down to $<30\text{km}$, resulting in the total depth of the model, and subsequently the vertical extent of the modelled mush region, being significantly less than the depth over which reactive flow occurs in the mantle (Kelemen et al., 1995a,b; Jackson et al., 2018). A 1D model therefore provides a

reasonable approximation to the system dynamics and has thus been used in the thermo-mechanical modelling presented in this thesis.

The thermo-mechanical model uses a porosity-dependent viscosity for the matrix through which the melt segregates. The porosity dependency is described by equation 3.1 (Solano et al., 2012). The value of the exponent β in equation 3.1 was set in the model to be 0.5 (Connolly and Podladchikov, 1998). η is the matrix bulk viscosity (Pas), η_* is the effective viscosity, and η_0 is the effective matrix viscosity (Pas) (Solano, 2011). The viscosity of the matrix is independent of the strain rate (i.e. Newtonian) due to the assumption of matrix deformation via melt enhanced diffusional creep (Cooper and Kohlstedt, 1984; Ranalli, 1987; Solano et al., 2012). ϕ is the melt fraction and ζ is the matrix shear viscosity (Pas).

$$\frac{4}{3}\eta + \zeta = \eta_* = \eta_0\phi^{-\beta} \quad (3.1)$$

Conservation of mass in the one-dimensional thermo-mechanical model is given by equation 3.2 (Solano et al., 2012, 2014). Phase change in the model is accounted for by determining the bi-directional movement of melt and matrix relative to a fixed reference frame of the mixture (Jackson et al., 2003). This is given by the final term in equation 3.2 where χ is the static degree of melting and z is the distance (m) over which melt migrates (Solano et al., 2012). The time (s) is given by t and w_s is the matrix velocity (ms^{-1}).

$$\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial z}[(1-\phi)w_s] + \frac{\partial\chi}{\partial t} + \left(2 - \frac{1}{\phi}\right)w_s \frac{\partial\chi}{\partial z} \quad (3.2)$$

Conservation of energy in the 1D system is given by equation 3.3 (Solano et al., 2014). It can be seen that this is defined in terms of h , enthalpy (J), with k being the thermal conductivity of the system ($\text{WK}^{-1}\text{m}^{-1}$), ρ is the effective density (kgm^{-3}), T is temperature (K), and L_f is the latent heat of fusion (Jkg^{-1}).

$$\frac{\partial h}{\partial t} = \frac{k}{\rho} \frac{\partial^2 T}{\partial z^2} + L_f \frac{\partial}{\partial z}[(1-\phi)w_s] \quad (3.3)$$

Momentum conservation is given by equation 3.4 (Solano et al., 2012). ρ_s and ρ_l denote the solid and liquid densities. The term k_ϕ is the permeability (m^2) of the matrix, μ is the shear viscosity of the melt, and g is the acceleration due to gravity (ms^{-2}).

$$\eta_0 \frac{\partial}{\partial z} \left(\phi^{-\beta} \frac{\partial}{\partial z} w_s \right) = (1 - \phi)(\rho_s - \rho_l)g - \frac{\mu\phi}{k_\phi} w_s \quad (3.4)$$

With the permeability given by equation 3.5:

$$k_\phi = ab^2 \phi^{\alpha} \quad (3.5)$$

Where a is the grain radius (m), b is the permeability constant, and α is the permeability exponent as described by Solano et al. (2012).

The governing conservation equations are strictly only valid below the solid-liquid-transition point, where the system consists of a low melt fraction along the grain boundaries within a highly crystalline mush. However, the equations are used at all melt fractions due to the transient nature of high melt fractions within the system (Jackson et al., 2003; Solano et al., 2012, 2014).

3.5 Benchmark: one dimensional column

Before using the thermomechanical model of Jackson et al. (2018) a number of benchmarking tests were carried out to ensure that the model was able to closely match previous work. The first test carried out was to ensure that the mathematical formulation for melt segregation was able to produce comparable results to the numerical solution of a compacting boundary layer found by Richter and McKenzie (1984).

This early work was chosen due to its geometric simplicity and the analytical tests run by Richter and McKenzie (1984) on their solution to the compaction problem. The case of an initially homogeneous melt fraction was chosen due to its simple analytic solution over short time periods. Adaptations were made to the boundary conditions of the thermomechanical model in order to replicate the column modelled by Richter and McKenzie (1984). The system was non-dimensionalised using the character-

istic time and length scales modified from Richter and McKenzie (1984) and defined by Solano (2011) in his appendix.

Initially the column, where the vertical scale represents depth as positive upwards, was set at dimensionless time $t = 0$ with uniform dimensionless melt fraction of 0.1. It is important to note that the non-dimensionalisation of melt fraction by Richter and McKenzie (1984) means that the initial system had a true, dimensional melt fraction of 0.1 but that this was scaled, as can be seen in figure 3.5, to be equal to an initial non-dimensional melt fraction of 1. This effectively simulates a column where the temperature is instantaneously brought above the solidus temperature in a homogeneous manner throughout the entire column. The velocities of the matrix and melt were uniformly set to 0 ms^{-1} at dimensionless time $t = 0$. The downward flow of the matrix relative to the melt results in negative matrix velocities. The fluid was set to have a lower density than the surrounding matrix, thereby allowing buoyancy-driven melt segregation to occur, with the melt travelling upward with positive velocities.

The Boussinesq approximation was applied over the entire column such that the density difference between the matrix and melt was neglected in all terms except those involving gravity. The height of the column was defined, as per Richter and McKenzie (1984), as being 50 non-dimensional characteristic length-scales, or compaction lengths. Compaction length is defined as depending only on the material properties of the matrix and the melt (McKenzie, 1984, 1985, 1987). More specifically, the characteristic compaction length is the distance from the lower, impermeable, compacting boundary within the vertical column over which compaction occurs (McKenzie, 1984). The uppermost surface of the impermeable matrix defines the compacting regime, as described in figure 3.4, and no solid flux occurs over the boundary.

The compacting boundary layer thickens with time to compensate for the volume of melt leaving. The rate of matrix deformation depends on the imbalance between the fluid pressure and the compacting lithostatic pressure in the column. The governing equations for a system involving bi-directional flow in partially molten material are derived from the equations for mass, energy, and momentum conservation from mixture theory (McKenzie, 1984). Darcy's law governs the buoyant flow of fluid along the pressure gradient.

The comparison between the results obtained by Richter and McKenzie (1984) and those produced by the thermomechanical model used in this thesis are shown in figure 3.5. It can be seen that the thermomechanical model is able to match the solution found by Richter and McKenzie (1984) very

closely across all three modelled parameters - melt fraction (3.5a), matrix velocity (3.5b), and melt velocity (3.5c).

Non-dimensional melt fraction is set to be equal to 1 at the start of the modelling (time $t = 0$) throughout the column. It can then be seen in figure 3.5a that the melt fraction in the base of the column decreases rapidly through time. The top of the column becomes fluid saturated, as can be seen by the decrease in height of the column containing melt fractions within the non-dimensional range of 0-1 from time $t = 2$ onwards. The column with initial non-dimensional melt fraction of 1 was initially 50 characteristic non-dimensional lengths in height and so, at time $t = 10$, the height of the fluid layer can be seen to be approximately equal to 10 characteristic lengths. This results in a decrease in melt fraction throughout the rest of the column as melt is slowly squeezed out and segregates upwards into the high melt fraction layer.

The results show good agreement between the numerical solutions used for the compaction problem and suggest that the governing equations for compaction in the thermomechanical model are valid for the assumptions used. In particular, the Boussinesq approximation holds in this instance as the thermo-mechanical model is concerned only with movement of melt in the vertical direction. Additionally, the thermo-mechanical model uses the discretisation scheme laid out in Richter and McKenzie (1984) which allows for a fair comparison between the two results for melt segregation in a column. The full set of equations which govern the mechanics of the model used in this thesis can be found in Solano et al. (2014).

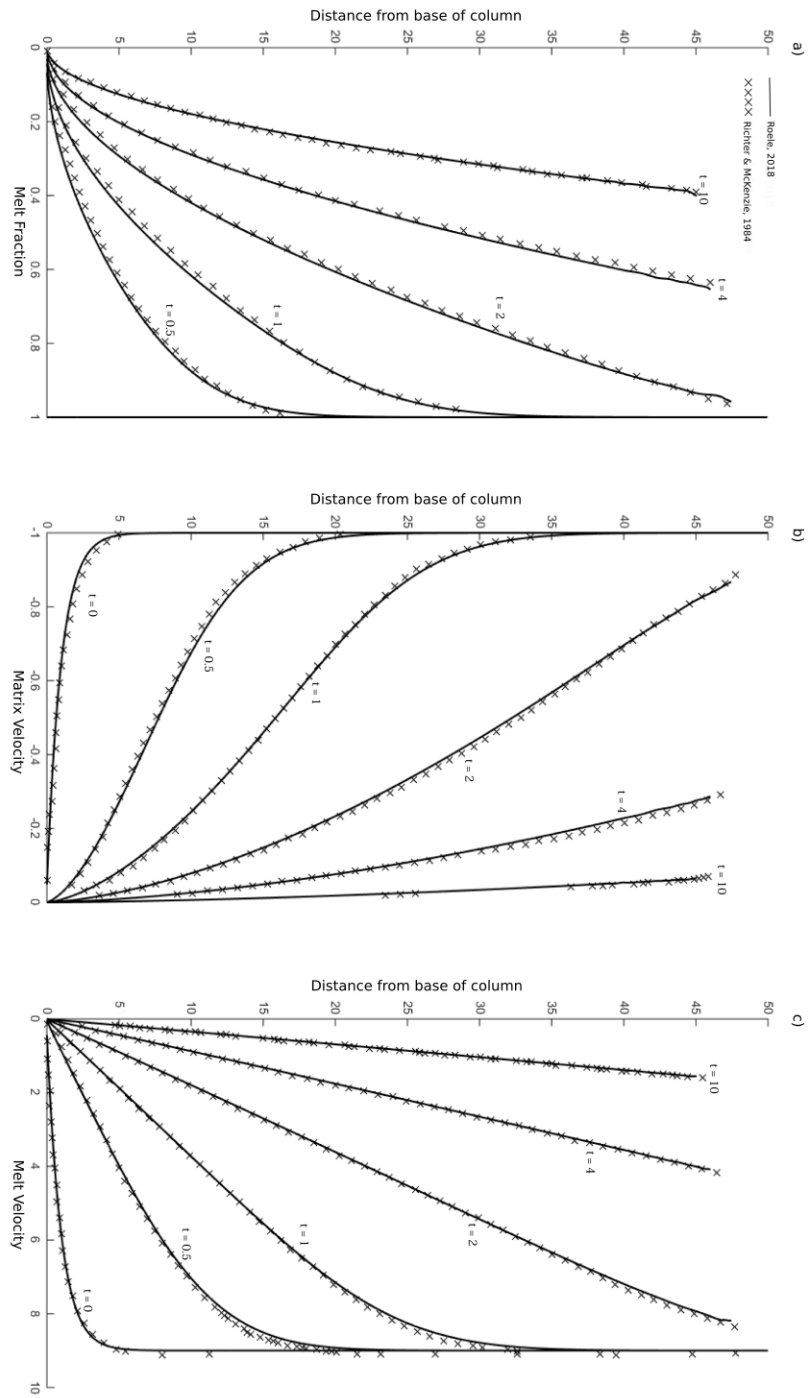


Figure 3.5: Comparison between the results of Richter and McKenzie (1984) and those obtained by the thermomechanical model used in this thesis for reactive flow in a compacting column. The solid lines are the results obtained with the thermomechanical model and the crosses show the results of Richter and McKenzie (1984). a) shows the non-dimensional melt fractions, b) shows the non-dimensional matrix velocity, and c) shows the non-dimensional melt velocity calculated throughout the column over non-dimensional time.

3.6 Benchmark: deep crustal hot zones

The second benchmark test carried out to validate the thermo-mechanical model was for the numerical solution of thermal diffusivity. In this case a comparison has been made against the results of a purely thermal model described by Annen et al. (2006). Their early model was developed in an attempt to better understand the generation of intermediate and silicic arc magmas. In particular, the model was aimed at determining the depth at which chemical differentiation occurred. Annen et al. (2006) assumed that the majority of chemical differentiation occurred in the deep crust based on the lack of evidence for mafic cumulates in the shallow crust (DeBari and Coleman, 1989; Kay and Kay, 1993; Glazner, 1994).

The model emplaced basalt into the deep crust and the site of emplacement was referred to as a deep crustal hot zone, as depicted in figure 3.6 (Annen et al., 2006). The model addresses the problem of thermal diffusivity in the deep crust and tracks melt evolution due to partial melting of surrounding crustal rocks. Mantle-derived basaltic sills are injected at multiple depths at their liquidus temperature and are allowed to cool in the thermal model.

Repetitive emplacement of 50 metre thick sills every 10^4 years, to give a one-dimensional emplacement rate of 5mm/yr was used in the thermomechanical model to match the inputs used by Annen et al. (2006). In order to be able to compare the thermomechanical model results with those of Annen et al. (2006) the advection terms governing melt segregation were turned off. The sills were emplaced at a depth of 20km to match the shallowest simulation run by Annen et al. (2006) at the Conrad Discontinuity. While the deeper models could also have been used as a benchmarking test this would have involved a much longer computation time due to the greater extent of the domain and the serial nature of the model, as both the deep and shallow thermal models in Annen et al. (2006) had a simulation run time of 16Ma.

When analysing the results of the thermo-mechanical model against those of the purely thermal model developed by Annen et al. (2006), it is important to note that the melting relationships used in the two models are not directly comparable. The thermomechanical model uses a simple binary eutectic phase diagram to determine the chemical composition of the melt and the matrix whilst maintaining local thermodynamic equilibrium in the system. A quadratic function was initially determined by Solano et al. (2014), and also used by Jackson et al. (2018) to describe the binary phase diagram which has been used in this thermo-mechanical model and is shown in table 3.1.

The melt fraction in this instance is then related to the liquidus and solidus compositions by equation 3.6. The solid composition, C_S , is bimodal and can take a value of either 1, the least evolved, or 0, the most evolved, as shown in table 3.1. In practice, only solid compositions corresponding to the most evolved state were used. This is defined as being where the local bulk composition, C , is less than a pre-determined value, e (the eutectic composition), as shown in table 3.1. The constants a_1 - a_3 used in the quadratic equation for the liquid composition in the binary phase diagram were chosen to represent the country rock and intruding sills based on experimental data as described in Solano et al. (2014).

$$\phi = \frac{C - C_S}{C_L - C_S} \quad (3.6)$$

Where ϕ is the melt fraction, which takes a non-dimensional value, and C is the local bulk composition.

In contrast, the purely thermal model uses two linear relationships between melt fraction and temperature based on two different sets of experimental data points, at different temperatures and pressures, that have been spliced together. The low-temperature relationship used by Annen et al. (2006) and in subsequent thermal models is linear between the solidus temperature and a fixed temperature value, T_a , which is defined as the temperature at which crystallisation of amphiboles starts to occur. This section of the melting relationship is based on experiments carried out on basalt from the Cascades mountain range by Sisson et al. (2005), where granitic and rhyolitic melts were generated from H_2O rich basaltic compositions (H_2O of 1.7-2.3 wt%). The second, high-temperature linear relationship is fitted between T_a and the liquidus temperature as shown in table 3.2 (Annen et al., 2006; Annen, 2009, 2011; Annen et al., 2014). The melting relationship above T_a is based on experimental data on amphibolite melting collected by Müntener et al. (2001) on basaltic andesite, also from the Cascades mountain range.

The second fundamental difference in the calculations between the thermal model and the thermo-mechanical model is the relation between melt viscosity and dimensionless silica content in the thermo-mechanical model. The thermal model does not parameterise the SiO_2 content due to insufficient experimental data (Annen et al., 2006). As such, the composition of the melt is not tracked and only a basic indication of melt composition related to the melting relationship is given. Conversely, the

silica content of the molten phase in the thermo-mechanical model is linearly related to the logarithm of the melt viscosity, μ , as described by Solano et al. (2014) and Jackson et al. (2018). The melt and matrix viscosities relate directly to the melt fraction and composition of the melt throughout modelling in the thermo-mechanical model.

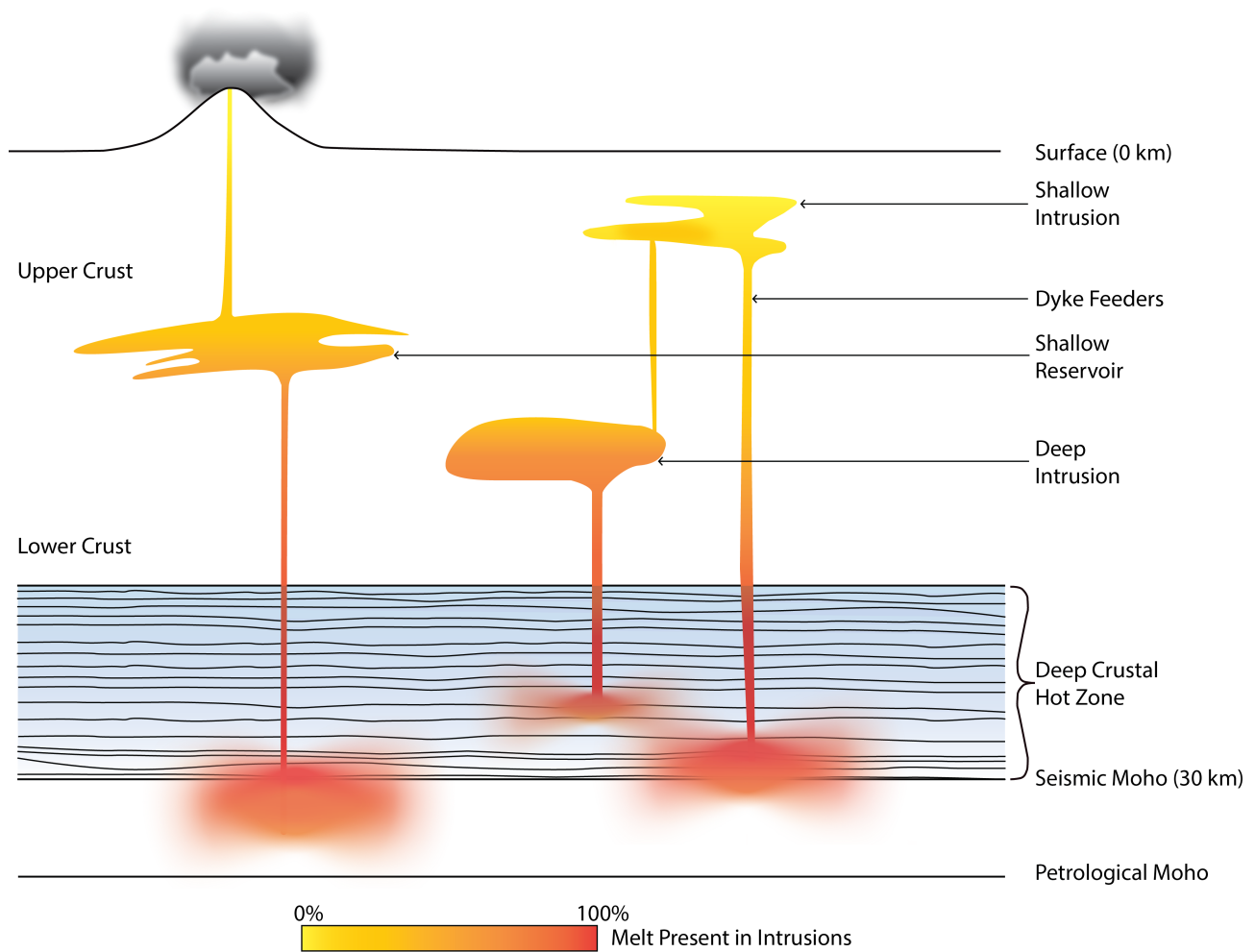


Figure 3.6: Adapted from Annen et al. (2006). Not to scale. Representation of a deep crustal hot zone where mantle-derived basaltic sills are emplaced in the deep crust at discontinuities. The influx of hot material melts the surrounding crust leading to further rise of melt into shallow magma chambers through sub-volcanic systems.

C Liquidus or Solidus	Composition	Validity
C_L	$\frac{-b_1 - \sqrt{(b_1)^2 - 4a_1(c_1 - T)}}{2a_1}$	$C < e$
C_L	$\frac{-b_2 - \sqrt{(b_2)^2 - 4a_2(c_2 - T)}}{2a_2}$	$C > e$
C_S	0	$C < e$
C_S	1	$C > e$

Table 3.1: Adapted from Solano et al. (2014). During modelling, only compositions C less than e were used. The values of constants a_1 - c_2 were chosen to relate to typical experimental data for both intruded basalt and the surrounding crust (Solano et al., 2014). The values for C_L and C_S are determined using the quadratic equation for the binary phase diagram and then substituted into equation 3.6 to determine the melt fraction, ϕ , for any given temperature value, T .

where $a_1 = -466$, $b_1 = -135.69$, $c_1 = 1826.5$

and $a_2 = -93.75$, $b_2 = -484.32$, $c_2 = 275.2$

as determined by Solano et al. (2014) who fitted a quadratic to experimental data obtained by Weill et al. (1980).

Temperature Range	Melt Fraction
$T \leq T_S$	0
$T_S \leq T \leq T_a$	$3.25 \times 10^{-3}(T - T_L) + 1$
$T_a \leq T \leq T_L$	$\frac{X_a}{T_a - T_S}(T - T_S)$
$T \geq T_L$	1

Table 3.2: Adapted from Annen et al. (2006). The melting relationship was chosen to match the experimental data of Sisson et al. (2005) between the solidus temperature and T_a , defined as the temperature at which amphibole is produced. T_S was 720°C and T_a was set to be 1040°C, based on the data of Foden and Green (1992). The relationship between melt fraction, X , and temperature above T_a was defined by data from Petford and Gallagher (2001). The liquidus temperature, T_L , was set at 1261°C based on the experimental work of Müntener et al. (2001).

Symbol	Unit	Description	Value
ρ_m	kgm^{-3}	Density of emplaced basalt	2830
C_{pm}	Jkg^{-1}	Specific heat capacity of emplaced basalt	1480
L_m	$\text{Jkg}^{-1}\text{K}^{-1}$	Specific latent heat of emplaced basalt	3.5×10^5
k	$\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$	Thermal conductivity of the entire system	3.0

Table 3.3: Adapted from Annen et al. (2006), parameters for the thermal model.

Figure 3.7 shows a comparison between the results from the model of Annen et al. (2006) and the thermo-mechanical model for the case of mantle-derived basalt intruding into pelitic and greywacke crust. Table 3.3 defines the parameters used for this benchmarking exercise, based on Annen et al. (2006). While the thermal model splits the crust into three regions; upper crust, emplacement zone, and lower crust, the thermo-mechanical model only defines the intruding material and surrounding crust. This leads to further differences in the final results, particularly at the boundary of the emplacement zone where the melting behaviour differs due to the different compositions used in the models. The general shape can be seen to be similar, particularly in the temperature results shown in figure 3.7a-c. Melt fractions shown in figure 3.7d are much lower than those calculated by Annen et al. (2006). This is due to the different melting relationship, outlined in tables 3.1 and 3.2. The general behaviour however can be seen to be similar, with high melt fractions at the top of the system and a low melt fraction column at the base of the system relating to the region of the crust where temperatures have increased above the solidus due to the heat flux from repetitive sill emplacements.

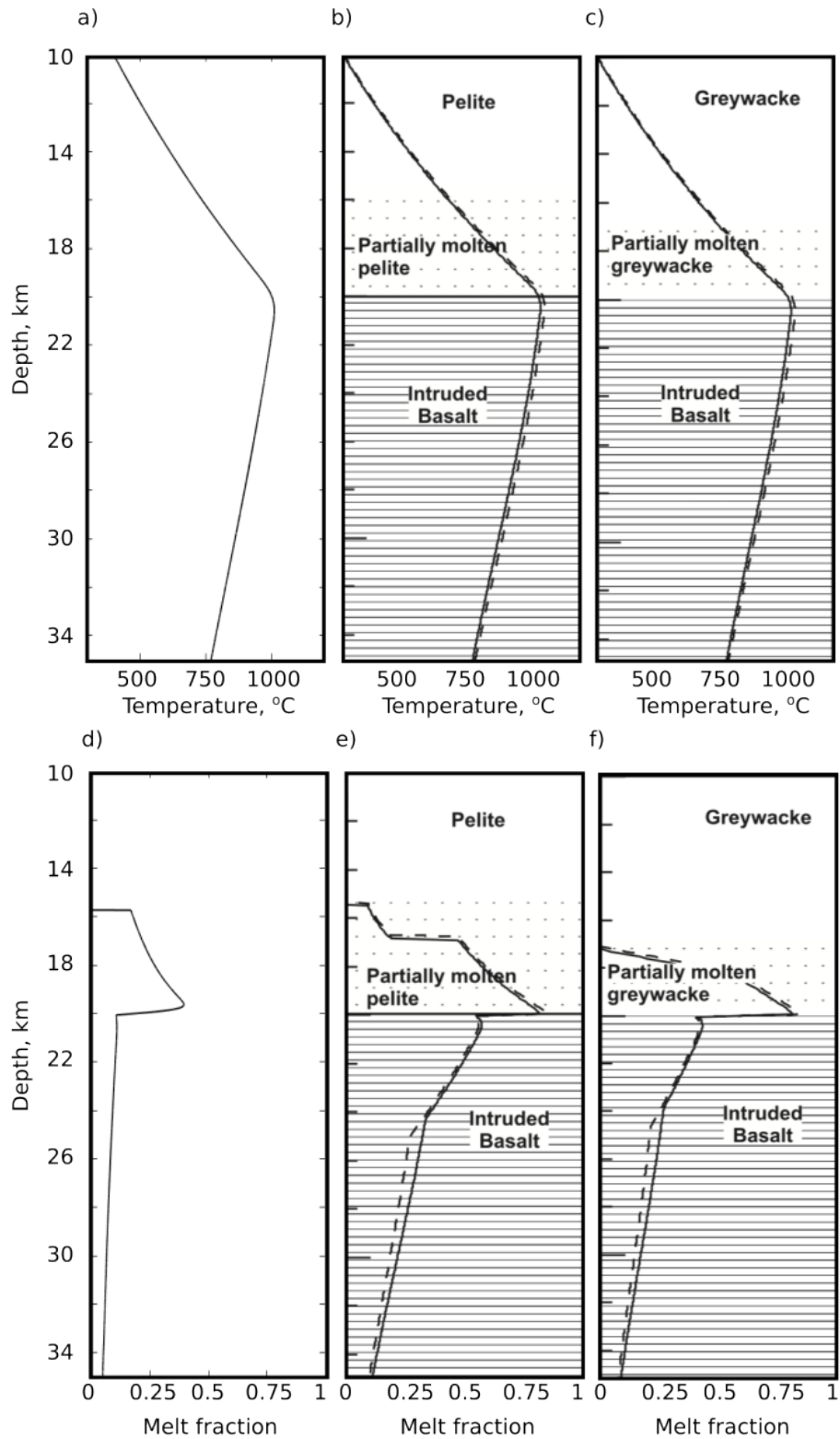


Figure 3.7: Adapted from Annen et al. (2006). a) Temperature results of the thermo-mechanical model used in this thesis, b) and c) temperature results of the thermal model for pelite and greywacke country rocks respectively. d) Melt fraction results of the thermo-mechanical model, e) and f) melt fraction results of the thermal model for pelite and greywacke country rocks respectively.

3.7 Benchmark: thermo-mechanical modelling

The thermomechanical model was initially run using the same inputs as in Jackson et al. (2018) in order to verify that the same results were obtained. The material properties can be found in table 3.4. These results are shown in figure 3.8 and were simply used to demonstrate that the changes to the non-dimensionalisation of the model have not affected the thermo-mechanical solution. Two different output times have been plotted in figure 3.8 to show that the results of Jackson et al. (2018) for SiO_2 content, melt fraction, and temperature can be reproduced through time.

Symbol	Unit	Description	Value
a	m	Matrix grain radius	2.5×10^{-3}
b	none	Permeability constant	1/500
α	none	Permeability exponent	3
β	none	Viscosity exponent	0.5
η	Pas	Matrix shear viscosity	10^{16}
μ	Pas	Melt shear viscosity	10^4
ζ	Pas	Matrix bulk viscosity	10^{16}
k	$\text{WK}^{-1}\text{m}^{-1}$	Thermal conductivity	3
L_f	Jkg^{-1}	Latent heat of fusion	350000
ρ_s	kgm^{-3}	Density of matrix	2800
ρ_l	kgm^{-3}	Density of melt	2300

Table 3.4: Parameters used to benchmark against Jackson et al. (2018).

As can be seen in figure 3.8 the final values for SiO_2 content, melt fraction, and temperature are the same when the same input values are used as in Jackson et al. (2018). The model was allowed to run for 2 Ma. Over accretion was used at an emplacement depth of 18.5 km. The first set of results shows a high melt fraction layer beginning to accumulate after repetitive emplacement of 50m thick sills over 1 Ma at a one-dimensional emplacement rate of 5mmpa with sills emplaced every 10ka. As can be seen from the second set of results at 1.99 Ma, the system was allowed time to cool and the melt fraction returned to zero after the temperature fell below the solidus along the entire 1D profile. It is clear from the SiO_2 data however that the melt migrated upwards, producing a more silicic layer at the top of the system, shallower than the initial input depth.

The adaptations made to the thermo-mechanical model have not changed the way in which the enthalpy method is implemented. As such, enthalpy is assumed to be released linearly during melting and is related to temperature through equation 3.7 as outlined in Solano et al. (2014). This results in the solution to the system of general equations remaining the same as in Solano et al. (2014) and a full description can be found in the appendix of Solano (2011). There have also been no changes to the binary eutectic phase diagram used to solve for the evolution of the melt and matrix compositions. This can be seen from the results for the SiO_2 content through the 1D domain. The spatial and temporal evolution of the SiO_2 content, melt fraction, and temperatures are therefore found to be identical in the two models. Determination of SiO_2 content and trace element concentration are calculated as described in Solano et al. (2014) equations 9 - 12.

$$h = c_p T + L_f \phi \quad (3.7)$$

At the base of the system, minor oscillations are visible in the SiO_2 content below 19km depth for the case at 1000 ka and below 22km depth for scenario shown at 1990 ka. These oscillations are also seen in the results of Jackson et al. (2018) and are due to the numerical approach used (Jackson, 2017, personal communication). The oscillations do not substantially increase over time and as a result can be assumed not to affect the numerical solution to the extent that it would inhibit analysis of the results (Jackson, 2017, personal communication). The small melt fraction waves with a moderately high frequency in the scenario shown at 1000 ka can be seen to be a true representation of the mechanics of the system by the number of data points along each wave. The grid spacing used throughout this thesis for the thermo-mechanical modelling is only 5 metres, which is well below the

minimum required by testing of the grid resolution shown in the following section. As a result these waves are considered to be real and not simply numerical. The high contrast in melt fractions across a relatively small physical space results in steep boundary conditions for the seismic problem discussed in later chapters.

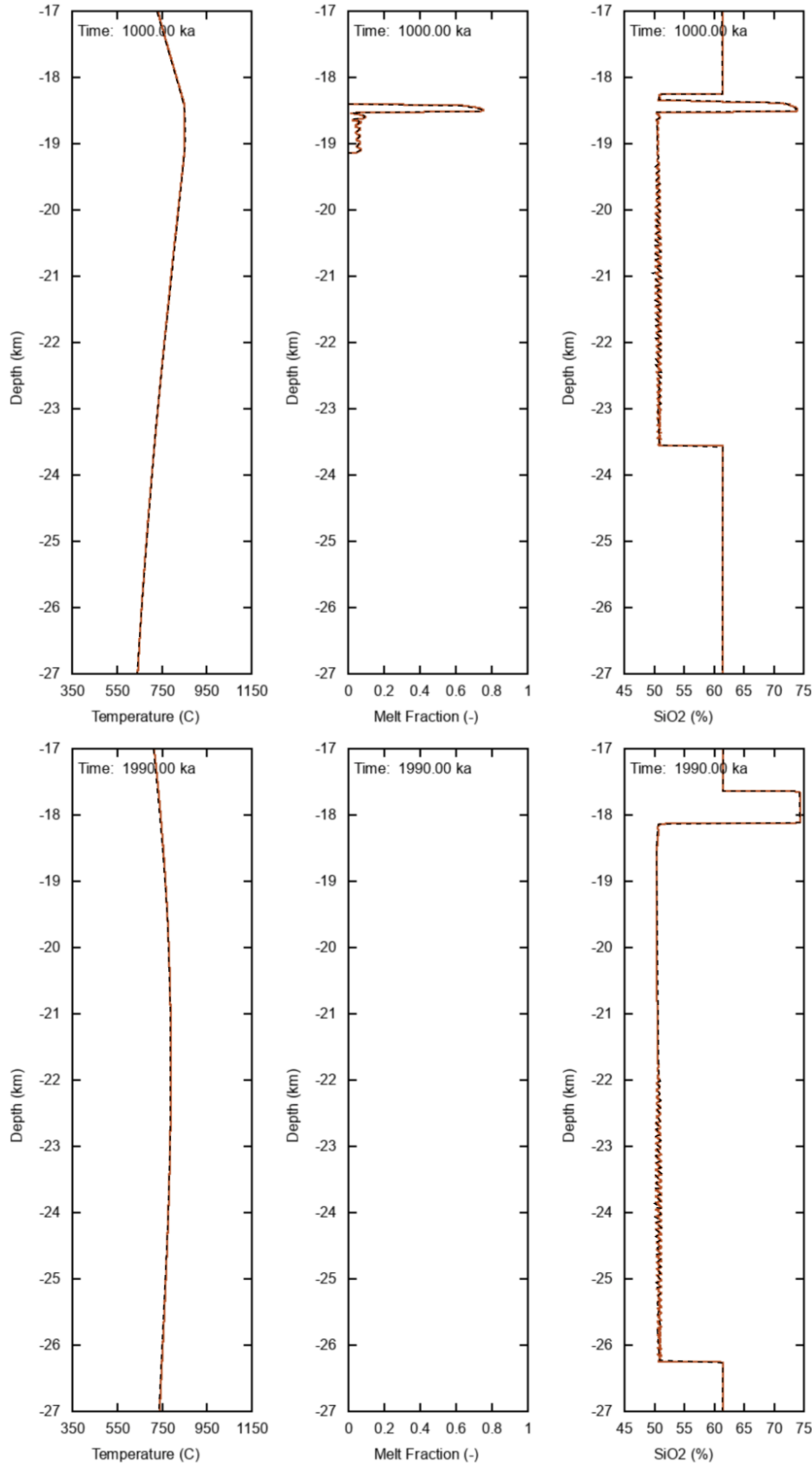


Figure 3.8: Adapted from Jackson et al. (2018). The solid orange lines show the results obtained by Jackson et al. (2018) while the dashed black lines show those obtained by the model used in this thesis. Two different time steps are shown - one half way through a 2 Ma long run after a 50m thick sill has been emplaced and allowed to cool for some time. The second set of results is at the end of the model run time after the system has been given time to cool. Initial SiO₂ was set at 61% for the country rock and 50% for the sills.

3.8 Grid resolution study

A final set of tests was run on the thermomechanical model to investigate the sensitivity of the grid and the number of time-steps used. Results of the grid resolution study are shown in figure 3.9 and results of the time-step study are shown in figure 3.10.

The thermomechanical model was set to have a grid spacing of 5 metres for all results shown in this thesis. In the grid resolution study presented in figure 3.9 the spacing between the nodes in the grid was initially halved and then doubled for the same input parameters to determine whether the solution was sensitive to grid spacing. As can be seen in figure 3.9, which shows the results of the grid resolution study for both temperature and melt fraction values, the solution matches very closely for 5 metre and 2.5 metre node spacing.

For the case where the grid size was doubled to 10 metres there is a clear difference in the calculated values for melt fraction however the difference is less apparent in the case of temperature. Fractionally higher temperatures are observed at depths greater than 22km in the sill emplacement zone for the case of 10 metre node spacing. This marginal increase in the temperature solution is enough to cause a large variation in melt fractions at these depths. Clearly there is therefore some sensitivity to mesh spacing in the final solution however the spacing used throughout this thesis of 5 metres between nodes can be seen to be well refined.

It is also clear from the graph showing sensitivity of the melt fraction results to grid spacing that instabilities occur in the solution at points of high gradients in melt fraction. However, it is clear that the convergence analysis yielded similar behaviour, suggesting the numerical method needs further research and development to remove these. It will be assumed throughout the rest of the thesis that the solution obtained by the numerical scheme is on average correct.

Results for the study determining the optimum value for the time step in the thermomechanical model are shown in figure 3.10. It can be seen that as the non-dimensional time step, δt , decreases, the solution becomes smoother. This is due to the importance of the higher order terms in the non-dimensionalised finite difference scheme. As both the time step and the grid spacing are refined, the error in the higher order terms reduces rapidly, since for the second order terms error reduces with the square of the grid spacing and time step, so halving either of these values reduces the error in the solution by a factor of four. As such, the higher order terms that have been retained in the explicit

finite difference scheme approximation to the solution, as laid out in Solano et al. (2014) and Jackson et al. (2018), produce a grid and time-step independent solution more rapidly than if the solution were simply a first order approximation.

The maximum size for the time step was determined using the Courant-Friedrichs-Lewy (CFL) condition as described in Courant et al. (1928). The CFL condition, equation 3.8, provides a maximum time step, δt based on the physical parameters in the model where u is the velocity of the melt, x is the grid spacing, and C is the Courant number. For explicit schemes such as that used in the thermo-mechanical model, $C_{\max}$ is equal to 1. The CFL condition is based on the principal that during advection, the time step must be less than the time taken for mass transport to occur between two points on a mesh with discrete spacing. In effect, the CFL condition provides a limit on the speed at which information can be propagated through the mesh. In order to achieve stability in the model solution, the CFL condition must be met. If the CFL condition (equation 3.8) is violated (i.e. δt is too large) the model moves faster than the maximum speed of information propagation through the model, rendering the system unstable.

$$C = \frac{u\delta t}{\delta x} \leq C_{\max} \quad (3.8)$$

While the CFL condition provides a necessary condition on the lower bound for the time step it is often not sufficient to provide stability on the final solution. As a result, the final value for δt used in finite difference schemes is often much smaller than that prescribed by the CFL condition. For the purposes of this thesis it was determined that a non-dimensional value of 8 time steps per CFL condition was optimal. While it would have been possible to run the thermo-mechanical model with an even smaller non-dimensional time step, the computational expense was deemed too high and outweighed the benefits from the smoother solution seen in figure 3.10. This is because the thermo-mechanical model runs in series and decreasing the time-step significantly increases run time. A small model domain of only 20 km in depth with a simulated run time of 1 Ma took approximately 12 hours to run with 8 non-dimensional time steps per CFL condition.

Figure 3.10 shows that the solution for the temperature equation remains constant across the range of tested time steps as this solution is not affected by the advection terms in the equation. The melt fraction solution however shows sensitivity to the time step used but it is clear from figure 3.10 that the differences are small. As such, the behaviour was deemed to be similar enough at 8 time steps per CFL condition to choose this value for δt when running the models.

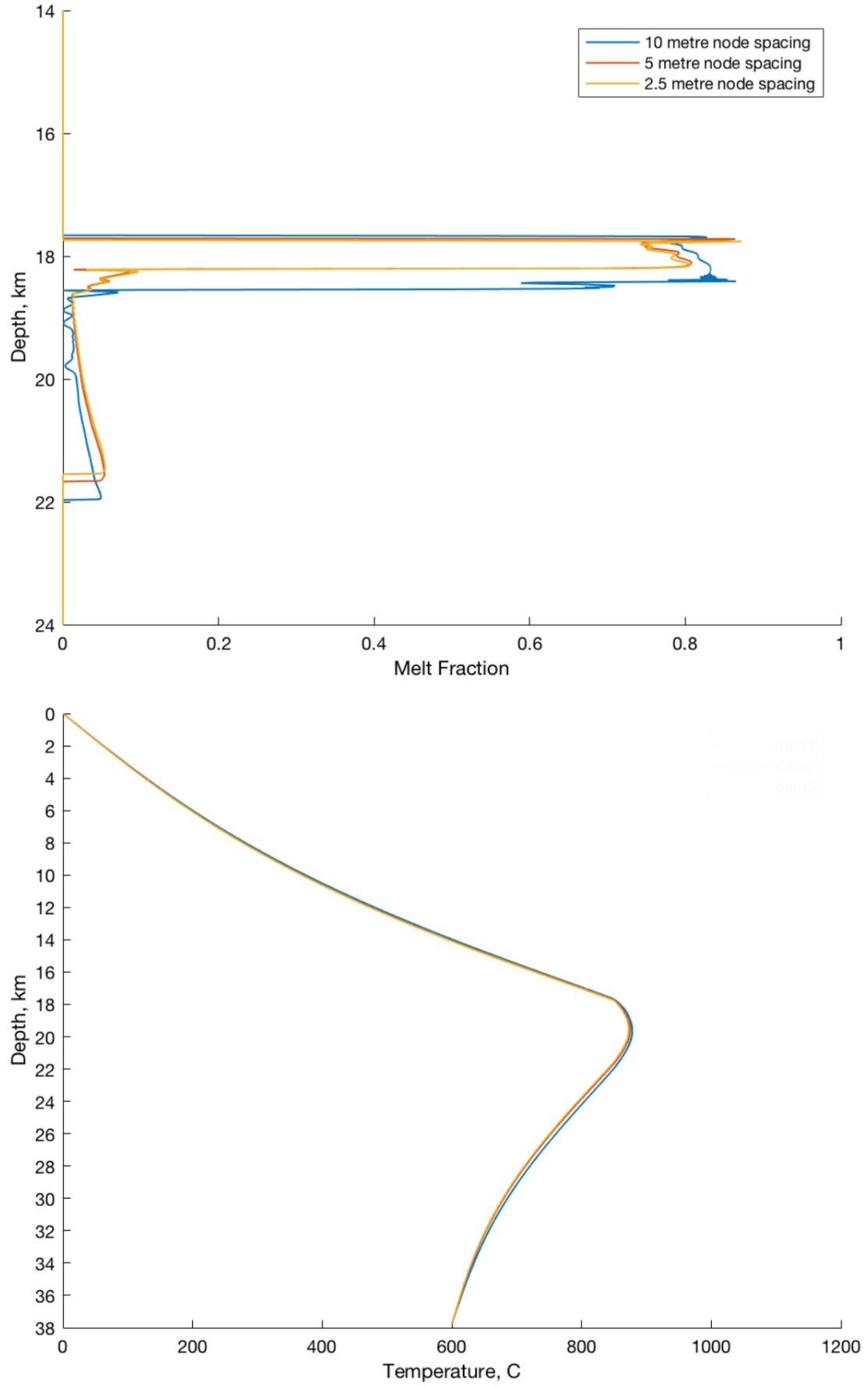


Figure 3.9: Grid resolution study carried out on the thermo-mechanical model for the case including segregation. This thesis used node spacing of 5 metres. Results for both halving and doubling the node spacing are presented.

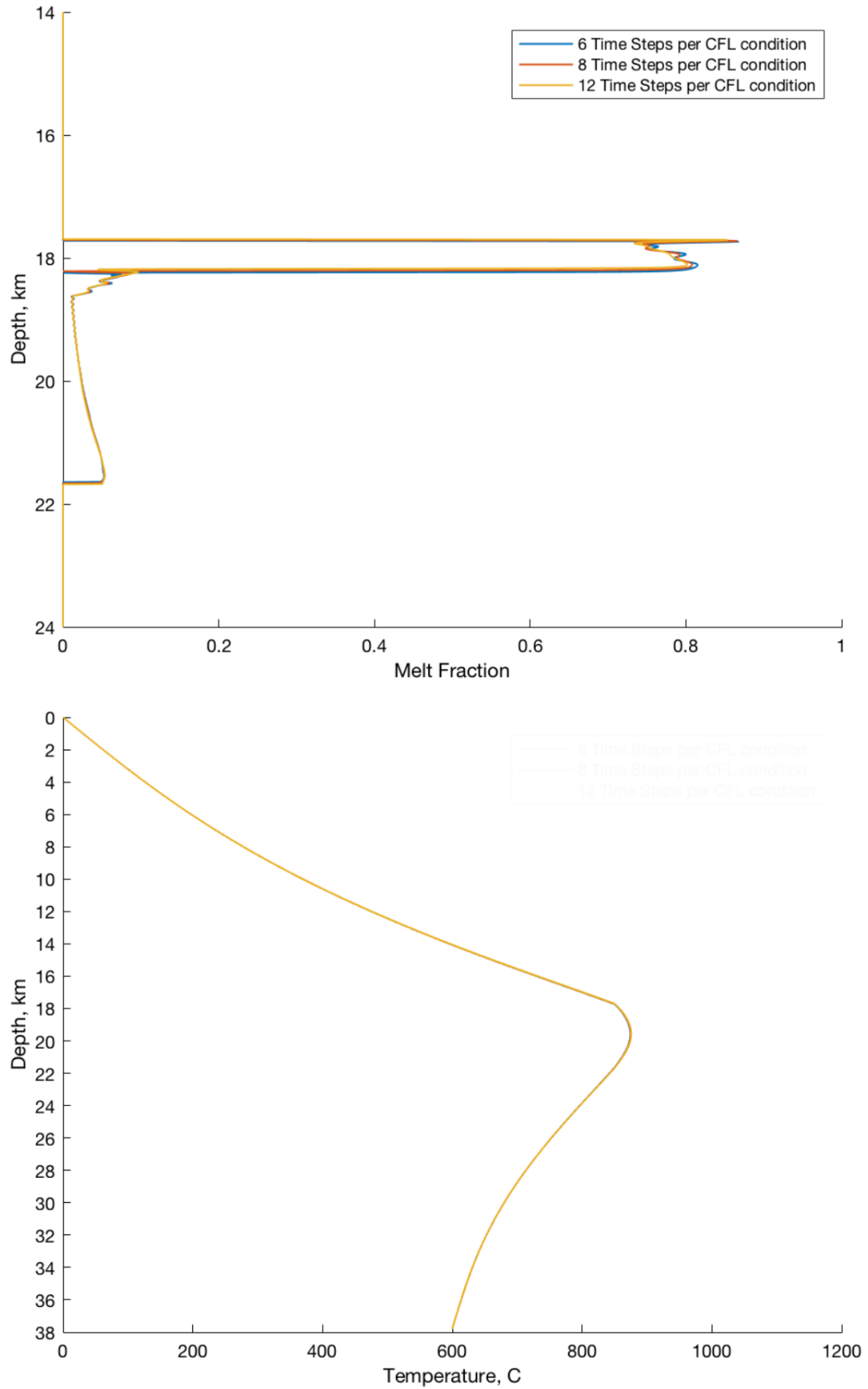


Figure 3.10: Test on the dependence of the solution in the thermo-mechanical model, for the case including segregation, on time step size. This thesis used 8 time steps per CFL condition.

3.9 Modelling carried out

A number of scenarios were modelled both with and without melt segregation to investigate the effect that including melt segregation in the governing equations has on the evolution of melt fraction distribution in the shallow crust. High, intermediate, and low emplacement rates were modelled to ascertain the extent to which high melt fractions are able to be sustained in the shallow crust due to chemical evolution during melt segregation. One-dimensional sill emplacement rates as high as 100 mmpa were used initially to simulate the high emplacement rates during dyke transport (Clemens and Mawer, 1992; Rutherford and Hill, 1993; Petford et al., 1996; Coleman et al., 2004). Emplacement rates were then progressively lowered to investigate how this affected the generation, storage, and evolution of the melt in the shallow crust. Comparisons were then drawn between the thermal and thermo-mechanical runs of the model to show the impact that including melt segregation and reactive flow has on the spatial and temporal evolution of melt distribution during modelling.

The 1-D emplacement rates used were 100 mmpa, 25 mmpa, 10 mmpa, and 5 mmpa. Sills 50 metres thick were emplaced repetitively via under accretion for 100 mmpa and via over accretion for all of the modelled emplacement rates. Under accretion has not been shown below 100 mmpa because under-accretion at very low emplacement rates results in sills eventually being emplaced in the deep crust where the background geothermal gradient produced temperatures that were high enough to incubate the sills after millions of years. Due to the focus of the modelling in this thesis being in the shallow crust beneath active volcanic centres this method of sustaining high melt fractions was deemed inappropriate. The emplacement depth was therefore set to be 5 km for each individual sill during repetitive intrusion in the shallow crust with an initial geothermal gradient of $50\text{ }^{\circ}\text{Ckm}^{-1}$ to be consistent with Solano et al. (2014).

3.10 Results

Figure 3.11 is a comparison between the results of the thermo-mechanical model at an emplacement rate of 100 mmpa for a thermal run (a-d) and when melt segregation is included (e-h). 3.11a and e show the temperature profiles while panels b and f display the corresponding melt fractions at an output time of 10 ka. Mantle-derived basaltic sills were 50 metres thick and emplaced via under accretion. While the temperature profiles are very similar there is a clear distinction between the melt

fraction results. In the thermal model (b) the location of maximum temperature and the location of maximum melt fraction occur at the same depth (6 km).

In contrast, panel f shows a high melt fraction layer above a relatively low melt fraction mush column with the high melt fraction layer occurring at 5.4 km depth, well above the location of maximum temperature. The high melt fraction layer at the base of the system in panel b occurs where the last sill was recently emplaced. It is clear from the contrast in the SiO_2 % and trace element concentration results that chemical evolution has occurred in the thermo-mechanical model. The depth of the maximum melt fraction in panel f corresponds with the depth at which a large increase in silica content, from a background level of 50% for the intruding rock type to 73.5% in the melt lens, is seen in panel g.

Initial silica content of the country rock was set at 61% while that of the intruding sills was set to be 50%. The trace element concentration, in ppm, started with an initial value of 20 ppm. This can be seen to evolve during thermo-mechanical modelling where component transport generates compositional variations which result in evolution of local melt composition to produce melt that is enriched in incompatible elements (Solano et al., 2014). In contrast however, it can be seen to stay constant in the purely thermal modelling as mass transfer is not accounted for.

The output time of 10 ka shown in figure 3.11 was chosen as this is the time scale required for a persistent high melt fraction layer to form over the Solid-Liquid-Transition (SLT) at an emplacement rate of 100 mmpa. The time scale over which incubation occurs and the SLT is reached is very short in both the thermal and thermo-mechanical runs of the model. For this rate of intrusion the model eventually became flooded with melt over time due to the large quantities of melt entering the system and the large increases in temperature associated with each sill emplacement.

The same inputs were used to produce figure 3.12 but the sills were intruded via over accretion at a consistent shallow crustal emplacement depth of 5 km. The comparison between the thermal results for melt fraction via under (3.11b) and over (3.12b) accretion at 10 ka shows that the profiles are similar but almost reversed through approximately 5.9 km depth. The difference in the emplacement style results in a high melt fraction layer being produced in the thermal model at the top of the system in figure 3.12b. It can be seen however that the location of highest melt fraction in 3.12b still correlates with the location of maximum temperature in 3.12a at 5 km, the over accretion emplacement depth.

In contrast, the results from thermo-mechanical modelling show that a high melt fraction layer has accumulated at a shallower depth, with the location of highest melt fraction within this melt lens occurring at 4.85 km. This is within the country rock and therefore shows that the high melt-fraction layer has melted the country rock immediately above it despite the lower temperature in this region, as outlined by the melting relationship in table 3.1, due to the more felsic composition of the country rock.

Due to the recent emplacement of a sill at 5 km depth it can be seen in panel f that melt fractions are equal to unity here but only for the thickness of the recently emplaced sill (50 m). The melt in this region has a low silica content (51% as seen in panel g) as its chemical composition is still that of the intruding rock type. In contrast, the melt lens between 4.75 - 5.00 km results from melt that has accumulated in the region following buoyancy driven melt segregation and as such it has a much higher silica content of 72%. The thin sills have resulted in a large variation in silica content across the thickness of the emplaced pluton. At 100 mmpa a 50 metre thick sill is emplaced every 500 years, producing a 1.05 km thick pluton over the time scale shown, with the base seen to be at 6.05 km.

The thermo-mechanical modelling results show the major difference in results when melt segregation is accounted for and treated as a coupled phase change and phase transport problem through a highly crystalline, complex mush system. Efficient exchange of heat and mass at the phase boundaries results in the melt and crystals remaining in constant thermal and chemical equilibrium (Jackson et al., 2005; Solano et al., 2014). The component transfer leads to changes in the local composition, which is calculated at each time step in the model and updated to facilitate modelling of melt evolution during segregation (Solano et al., 2014). As a result, melt evolution can be seen to occur, with melt being produced and sustained below solidus temperatures at the top of the thermo-mechanically modelled systems. This is due to the trace element partitioning between crystals and melt that was formulated by Solano et al. (2014) and used in the thermo-mechanical model.

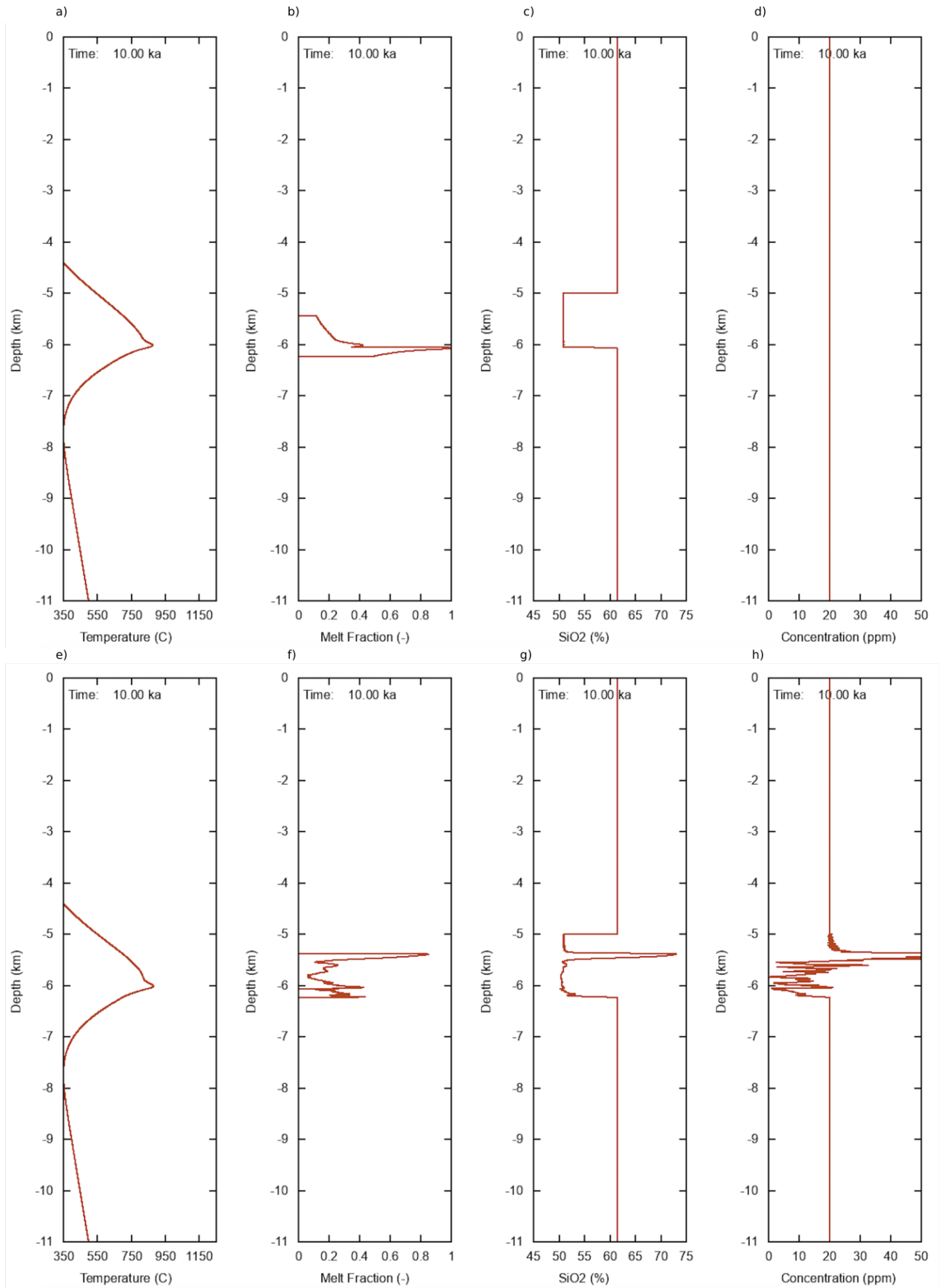


Figure 3.11: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 100 mmpa was used with a sill thickness of 50 metres emplaced via under accretion, results have been output after 10 ka.

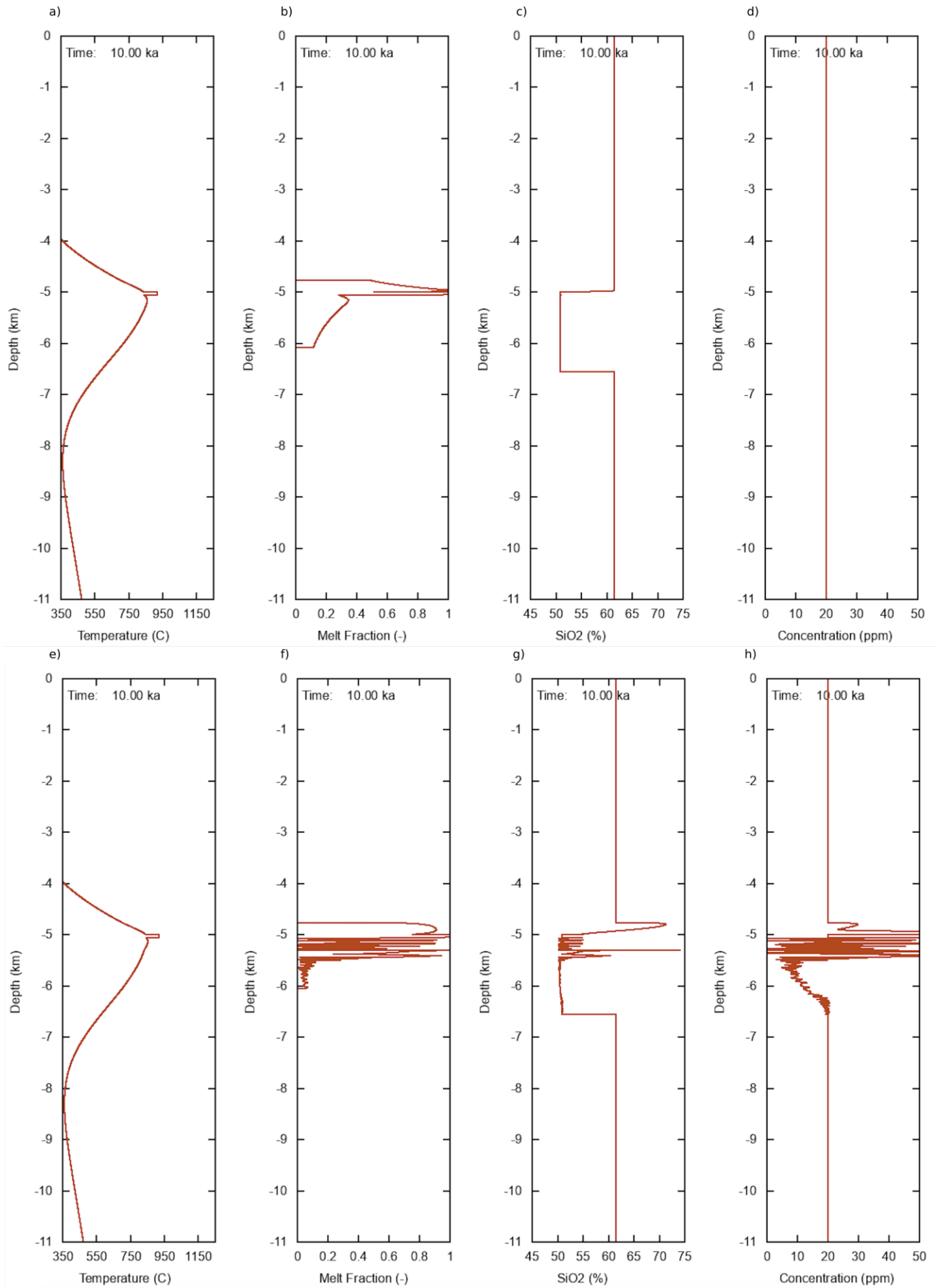


Figure 3.12: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 100 mmpa was used with a sill thickness of 50 metres emplaced via over accretion, results have been output after 10 ka, with the most recently emplaced sill visible at 5 km depth.

The region below the high melt fraction layer in the thermal results (3.12 b) decreases linearly from 0.4 at 5.2 km to 0.18 at 6.05 km and results from the temperature in this region being sufficiently above the solidus temperature to support the production of a small amount of melt in the system. In contrast, the region below the shallowest high melt fraction layer in the thermo-mechanical model (panel f) has much more variation in the resultant melt fractions due to the effects of chemical evolution and melt segregation. As melt migrates upward buoyantly it accumulates from depth into the observed shallow high melt fraction layer. This results in a much lower average melt fraction in the mush column (<0.1). The thin layers of high melt fraction seen between 5.0 and 5.4 km correspond to locations in panel g where the melt has evolved during migration and the solidus temperature has been lowered far enough to sustain melt generation.

Figure 3.13 shows a comparison between the results of a thermal (a-d) and thermo-mechanical (e-h) run of the model at an intermediate emplacement rate of 25 mmpa. The sill thickness was maintained at 50 metres and intrusions occurred via over accretion at a depth of 5 km with the most recently emplaced sill visible. While the temperature results of the two models are again very similar in figure 3.13a and e, there is a clear difference between panels b (without segregation) and f (with segregation) for the melt fraction distribution.

Both models have produced a large volume of eruptible magma with a sustained melt fraction well above the SLT. However, the thermo-mechanical model has accumulated significantly more melt, with a maximum melt fraction in the shallow melt lens of 0.91. In comparison, the maximum melt fraction in the thermal run of the model is only fractionally above 0.6. It can be seen from figure 3.13 that the location of maximum melt fraction in the thermal model again corresponds with the location of maximum temperature at 5 km whereas in the thermo-mechanical model these locations are decoupled and the maximum melt fraction is shallower at 4.87 km. The location of maximum melt fraction in panel f relates to the region of melt evolution where the percentage of silica is very high (72.5%). Melt is able to be sustained here at the lower temperature due to its chemical evolution during buoyant melt segregation through the mush column. The mush column has been depleted of melt in panel f compared to panel b due to melt migration. As a result, the mush column in the thermo-mechanical model displays a much higher average crystallinity throughout its thickness than in the thermal column where melt fraction is linearly related to temperature.

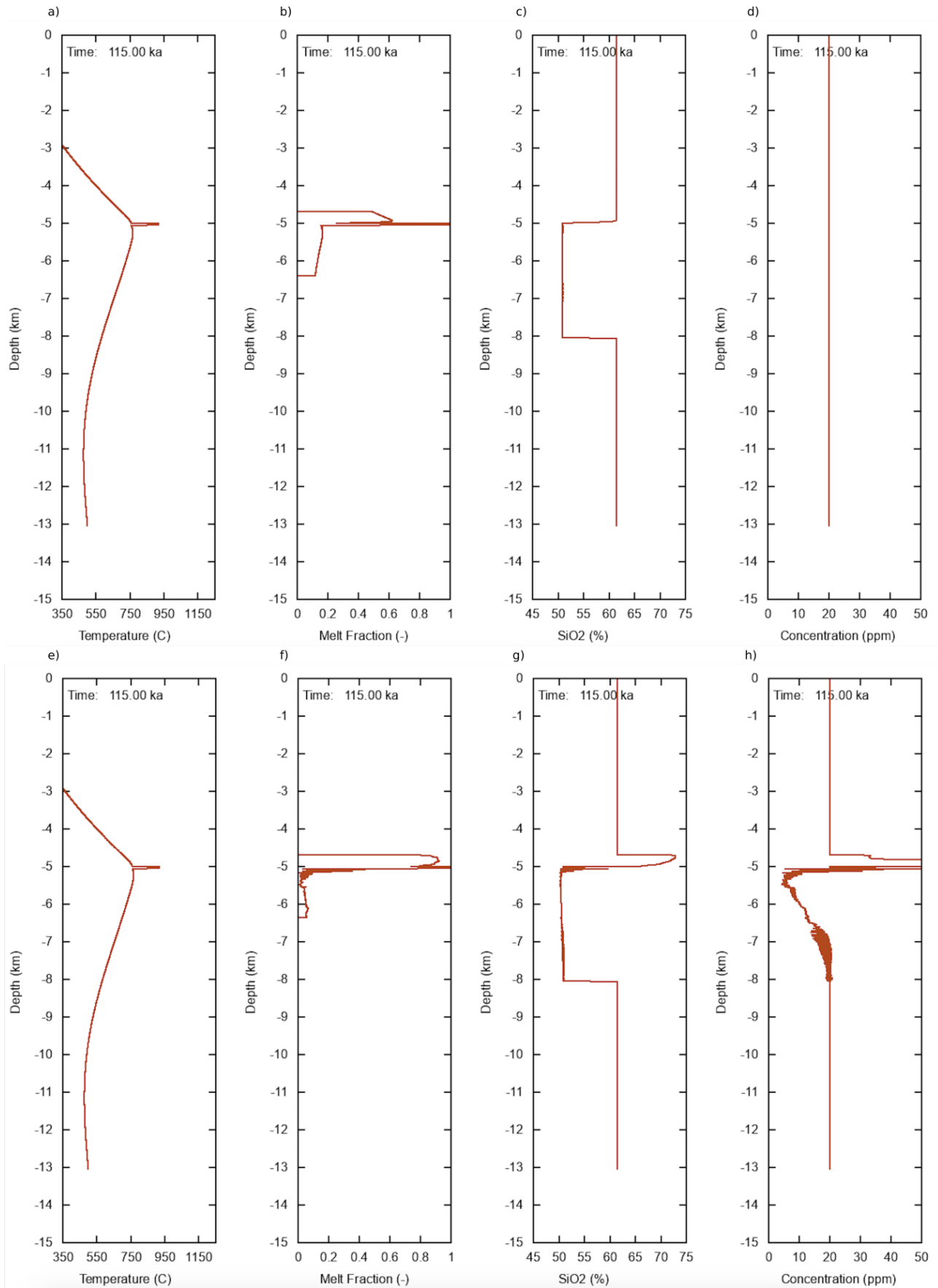


Figure 3.13: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 25 mmpa was used via over accretion with a sill thickness of 50 metres, results have been output after 115 ka with a pluton thickness of 2.8 km

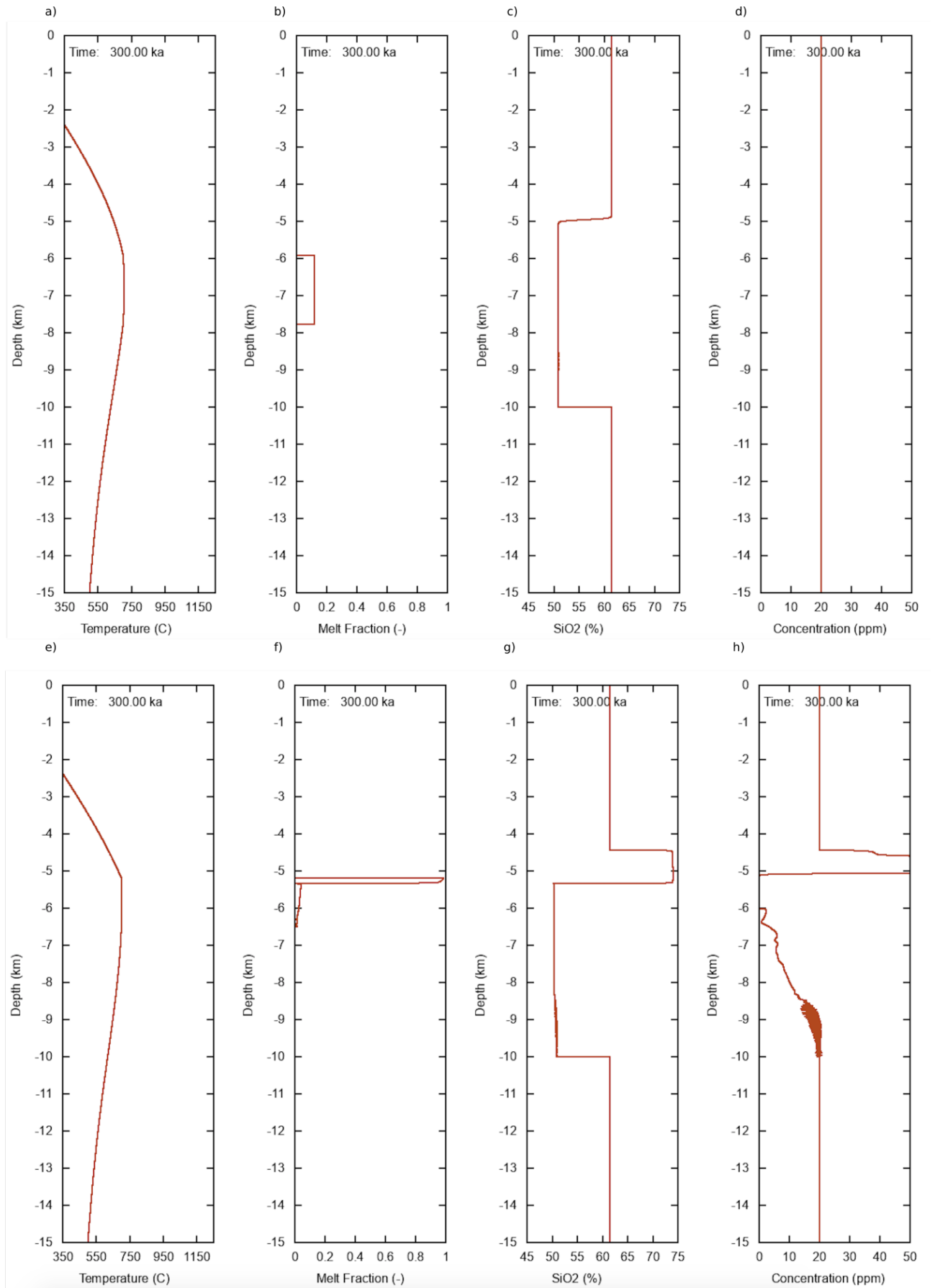


Figure 3.14: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 25 mmpa was used via over accretion with a sill thickness of 50 metres, results have been output after 300 ka. A pluton 5 km thick was emplaced over 200 ka.

A large difference can be seen in the results of the thermal and thermo-mechanical modelling when the system is allowed to cool substantially following the final sill emplacement. Figure 3.14 shows the same system as in figure 3.13 at an output time of 300 ka. The total thickness of the emplaced pluton was 5 km at a rate of 25 mmpa over 200 ka. The results in figure 3.14 therefore show the system after 100 ka of cooling. The comparison between panels a and e show that the temperature results remain fairly similar however a region of slightly elevated temperature is observed at 5.2 km. This relates to the location of a melt lens with a very high melt fraction of almost unity in the thermo-mechanical model (figure 3.13f). The melt lens seen in panel f corresponds to the region of high silica content in panel g (74%) and is bounded on the top surface by the location of the solidus isotherm (700 °C) in panel e. A very low melt fraction column is visible between 5.3 and 6.4 km depth in 3.14f which can be seen to have been depleted of incompatible trace elements in panel h. In contrast, the melt fraction distribution predicted by the thermal model in panel b shows a consistent low melt fraction (0.15) throughout the region where temperatures have not relaxed below the solidus. The melt fraction in the thermal model is not high enough to be classified as an eruptible volume of melt due to its high crystallinity however the (approximately 200 metres thick) melt lens in the thermo-mechanical model is sufficiently large and crystal-poor to be a mobile, eruptible magma.

Similar behaviour is observed at low emplacement rates as at intermediate rates, with the thermo-mechanical model able to sustain high melt volume fractions after cooling at low emplacement rates. However, it is important to note that lowering the emplacement rate results in a much longer incubation time. This is evidenced in figure 3.15 where an emplacement rate of 10 mmpa was used to accumulate a pluton 15 km thick over 1.5 Ma. The outputs in figure 3.15 are shown after 600 ka, with the most recent 50 metre thick sill visible at the over accretion emplacement depth of 5 km. Panels a-d show the results of thermal modelling while e-h show the results when melt segregation is included. At such a low emplacement rate the incubation time can be seen to have been very similar with both panels b and f showing a high melt fraction region where the most recent sill has been emplaced and a low melt fraction zone below where the crust has been incubated and a persistent low melt fraction has formed. The melt lens observed forming at the top of the system in the thermo-mechanical model is thicker than that in the thermal model as melt has segregated buoyantly and accumulated at the top of the pluton. As a result the low melt fraction mush column forming in panel f has a lower overall melt fraction than that in the thermal model in 3.15b.

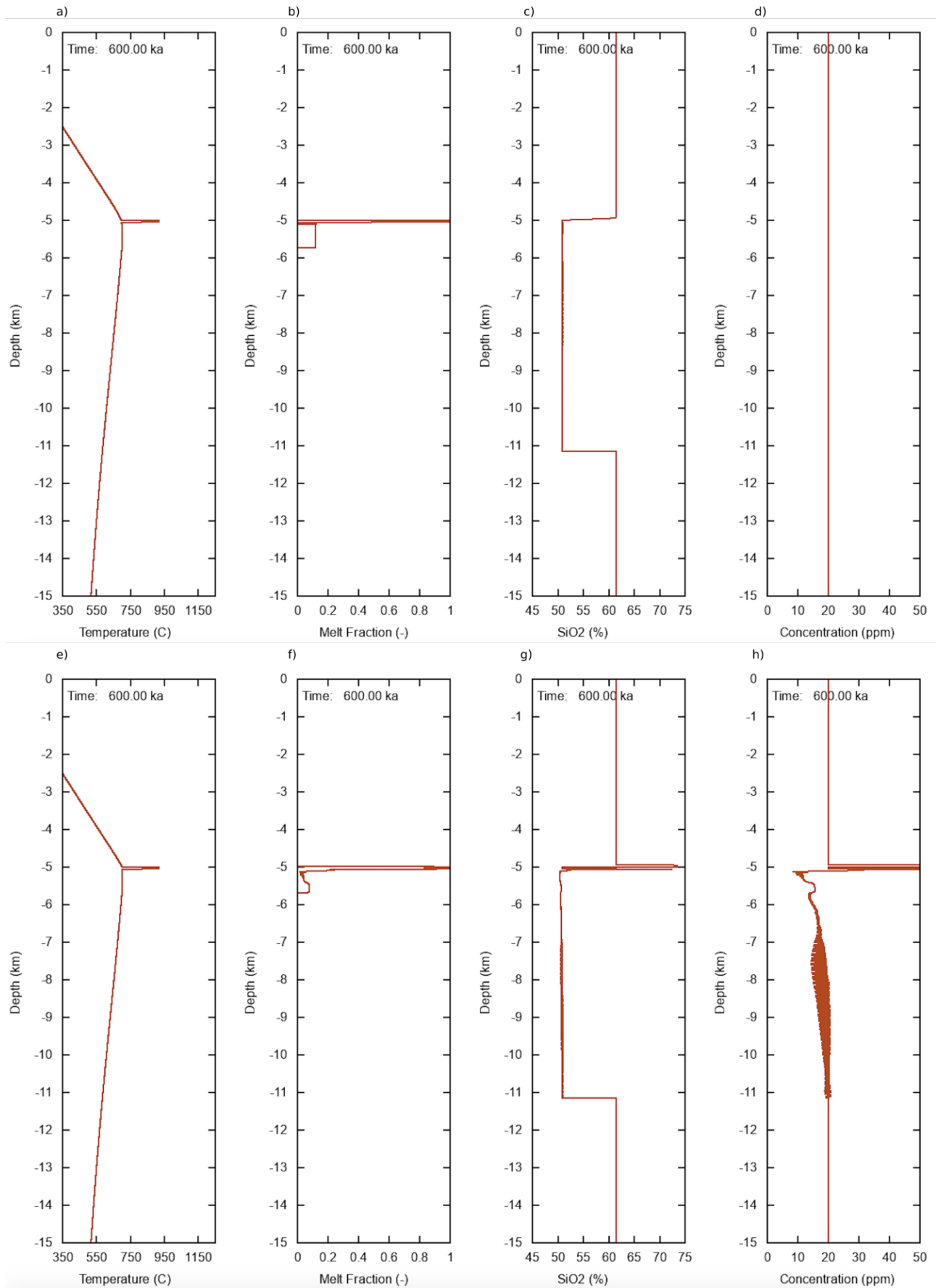


Figure 3.15: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 10 mmpa was used via over accretion with a sill thickness of 50 metres, results have been output after 600 ka with a pluton thickness of 6 km

As with intermediate emplacement rates the main difference in melt fraction distribution occurs once the system has been allowed to cool. Figure 3.16 shows the same system as in 3.15 after a total pluton thickness of 15 km was emplaced over 1.5 Ma and the system was allowed to cool for 10 ka. Although the temperature results remain similar for both the thermal (a-d) and thermo-mechanical (e-h) modelling results the melt fractions and silica contents show a very different evolution. The thermo-mechanical model can be seen in panel f to have sustained a large region of high melt fraction at the top of the system despite the cooling period. The location of the large melt volume corresponds to the region in panel g where silica content is greater than 74%. Whereas in the thermal model the linear relationship between temperature and melt fraction has resulted in a low melt fraction column in the region between 5.2 - 11.9 km where temperatures exceed the solidus, chemical evolution in the thermo-mechanical modelling has resulted in the location of maximum melt fraction not being aligned with the location of maximum temperature. In addition, the mush column observed in the thermo-mechanical model has a lower melt fraction (averaging approximately 0.07) than that in the thermal model (0.18) due to melt migrating through the system and accumulating in the shallow melt lens.

Modelling results using a very low emplacement rate of only 5 mmpa, with accretion of 50 metre thick sills via over accretion, are shown in figure 3.17. As can be seen from panels b and f the very low emplacement rate is not able to produce or sustain a body of melt in either the thermal or the thermo-mechanical modelling. 3.17a and e show that the temperature of the system remains below the solidus and as such the crust has not been incubated despite the model run time of almost 2 Ma producing an emplacement zone 10 km thick. The SiO₂ % and trace element concentration results show that evolution of melt occurred within each individual sill in the thermo-mechanical model, evidenced by the small-scale variations seen in silica content between 5 and 10 km depths and the very high percentage of silica observed at the top of the emplacement zone where new sills are emplaced via over accretion.

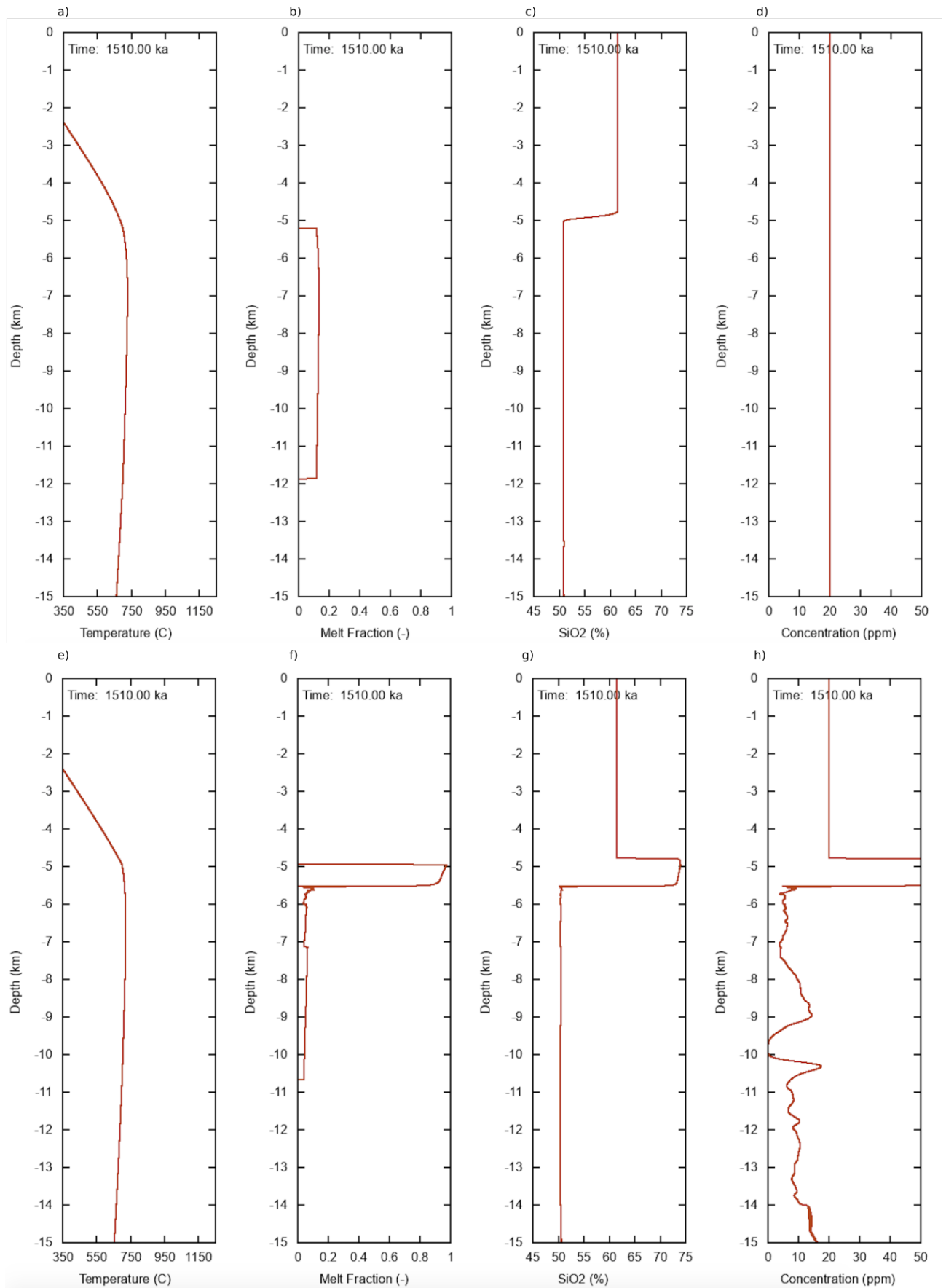


Figure 3.16: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 10 mmpa was used via over accretion with a sill thickness of 50 metres, results have been output after 1.51 Ma. A pluton 15 km thick was emplaced over 1.5 Ma.

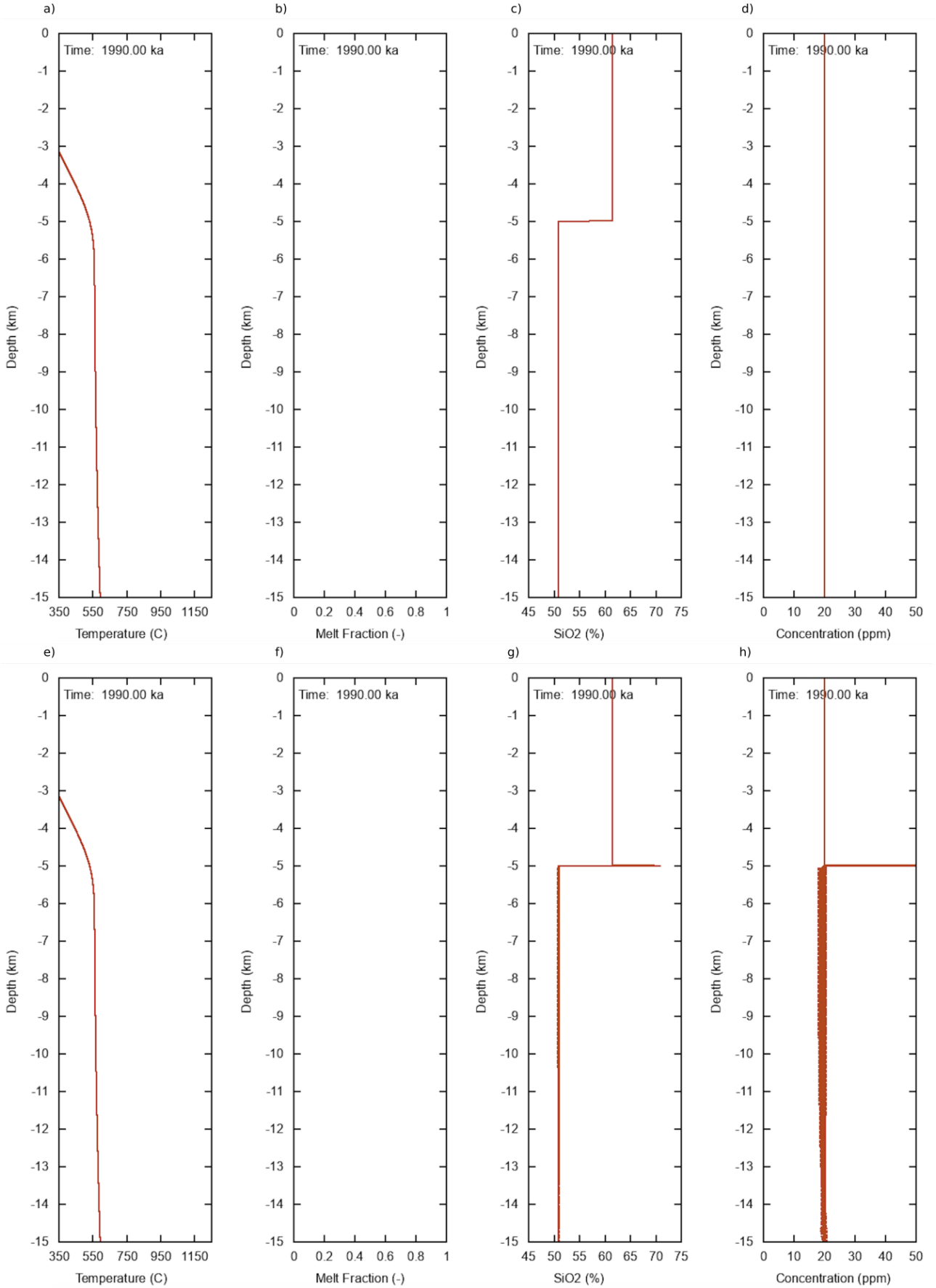


Figure 3.17: a)-d) Results using a thermal run of the thermo-mechanical model, e)-h) Results when melt segregation and matrix compaction terms are considered during thermo-mechanical modelling. An emplacement rate of 5 mmpa was used via over accretion with a sill thickness of 50 metres. A pluton 10 km thick was emplaced over 2 Ma.

3.11 Discussion

Results from thermo-mechanical modelling are consistent with previous thermal models when very low emplacement rates are used. The background temperature of the crust in both cases does not increase substantially for incubation to occur and so melt is not able to accumulate. This can be seen in figure 3.17 where emplacement occurred via over accretion and a rate of only 5 mmpa was used. The results for under accretion in this case were not shown as the pluton thickness eventually became so large that the sills were no longer being emplaced at shallow crustal depths.

The main difference in the results when melt segregation, matrix compaction, and reactive flow are included in the thermo-mechanical modelling is the production of a very low melt fraction 'mush' column as can be seen in figure 3.14 which can be sustained during periods of cooling. Whereas thermal modelling is only capable of producing high melt fractions through the addition of heat via sill emplacements, melt segregation allows the melt to migrate through the system while maintaining thermal and chemical equilibrium. This results in a much lower melt fraction (<0.1) in the region below the emplacement zone during over accretion as mobile melt migrates upwards along grain boundaries and accumulates in a high melt fraction lens in the shallow crust at cooler temperatures. When mass transfer is not included in the modelling the mush column maintains a higher average melt fraction compared to thermo-mechanical modelling (observed in figures 3.13b and 3.15b), however the region of highest melt fraction corresponds to the region of highest temperature, resulting in rapid crystallisation during cooling (figures 3.14b and 3.16b).

The chemical evolution of the migrating melt is evidenced by the change in SiO_2 % through the modelled emplacement zones. As silica content increases the region becomes more felsic and subsequently has a lower solidus temperature. This results in the production of the observed high melt fraction layers in the thermo-mechanical models that are not seen in the thermal models. Due to the chemical evolution of the melt during segregation away from the initial site of intrusion it is possible for high melt fractions to be sustained at low temperatures in the thermo-mechanical model. The mush column that forms during repetitive sill emplacements is therefore able to remain in a highly crystalline state without completely solidifying as silica content is increased from 50% in the emplaced melt to $>70\%$ in the highly evolved shallow melt lens. Additionally, the high melt fraction layers that form with high silica contents remain at the top of the system, bounded by the country rock solidus isotherm, and can be sustained during periods of cooling (figure 3.14e).

The results of the thermo-mechanical model show multiple high melt fraction layers which are similar to the compositional layers found in observations of migmatites (Sawyer, 1994, 1996; Brown, 1994). In addition, the trace element partitioning method used in the thermo-mechanical model has previously been shown to match well with observations of melt evolution during buoyancy-driven flow (Quick et al., 1992, 1994; Sinigoi et al., 1994; Solano et al., 2012, 2014).

It is important to note that the composition of the high melt fraction layers produced by the thermo-mechanical model relates to only a very small fraction of melting, as found by (Jackson et al., 2003, 2005; Solano et al., 2014). This is because the melt and surrounding rock maintain thermal and chemical equilibrium during melt segregation resulting in the melt equilibrating with the solid at progressively lower temperatures as it migrates upwards into the cooler crust. Constant evolution produces compositional stratification within the shallow crust, evidence for which is supported by geophysical observations (Jellinek and Kerr, 1999; Kellogg et al., 1999; Warner et al., 2013). In addition, the small degree of melting required means that large restite cumulates do not get left behind in the shallow crust during thermo-mechanical modelling which is also consistent with geophysical observations (Hanson and Glazner, 1995; Petford et al., 1996; Glazner and Miller, 1997; McCaffrey and Petford, 1997; Glazner et al., 2004).

3.12 Conclusion

At very low sill emplacement rates in the thermo-mechanical model, it is found that the maximum melt fraction remains well below that required to create an eruptible volume of magma. This result is consistent with static models published previously. However, at realistic intermediate sill emplacement rates (deemed as such based on observations of heat and magma fluxes at active volcanoes), the formation of a high melt fraction layer within a low melt fraction background is observed (Huppert and Sparks, 1988b,a; Hanson and Glazner, 1995; Spera and Bohrsen, 2004; Jackson et al., 2005). The high melt fraction layer produced via melt segregation migrate upwards toward the top of the mush column which is defined by the location of the solidus isotherm. Despite having a high melt fraction, the melt in the layer has a composition corresponding to a progressively larger degree of fractionation, producing a more felsic melt during upwards migration, because it locally equilibrates with the mush at progressively lower temperatures. Thus the composition of the melt in the high melt fraction layers becomes progressively more evolved, with higher silica content.

The high melt fraction layer produced at the top of the mush column in the thermo-mechanical model resembles a conventional magma chamber. However, it is important to note that it is produced by changes in bulk composition in response to melt migration, rather than the addition of heat, which is used in thermal modelling. Indeed, such a layer can form and be sustained even when the mush is cooling overall. The magma within the layer is at sufficiently high melt fraction to be eruptible, but is not located in the hottest region of the mush where the temperature is highest. This is in contrast with the results of thermal models where the region of highest melt fraction is coupled with the depth location of the highest temperature.

The results show that high melt fractions need not be associated with high temperature; they also show that eruptible melt fractions can be created at much lower emplacement rates than predicted by static models. These high melt fractions are transient, and spatially localised within larger mush zones. Moreover, chemical differentiation does not require fractional crystallisation in a largely liquid magma chamber. Thermo-mechanical modelling is consistent with recent geophysical, geochemical and petrological data that suggest crustal magma chambers are normally largely crystalline, with high melt fractions present only transiently prior to eruption (Jackson et al., 2003, 2005; Bachmann and Bergantz, 2006; Solano et al., 2012, 2014; Caricchi and Blundy, 2015a,b). The modelling provides quantitative estimates of volumes, rates and timescales for the formation of eruptible magma which can be integrated with data from active volcanic centres to investigate the spatio-temporal evolution of melt distribution.

Future work using the thermo-mechanical model could include a full 3D cylindrical model of the studied volcanic plumbing systems. This would provide a much more detailed and holistic understanding of the evolution of melt distribution. In addition, it would allow for a comparison between previous pseudo-3D static modelling and the results of the thermo-mechanical model, where lateral movement of melt could also be accounted for.

Chapter 4

Estimating Seismic Velocities

4.1 Background

In order to take the predictions of melt distribution made by the thermo-mechanical model and compare them with seismic data collected at active volcanic centres, an approach has been developed to convert melt fraction and temperature values in a 2D domain into seismic velocities. This has been done by following the procedure set out in Paulatto et al. (2012) who determined the potential contribution attributed to both temperature and the presence of melt for the velocity anomaly observed beneath the Soufrière Hills Volcano in Montserrat. Here, the method has been used to provide forward predictions of P-wave velocity for the modelled temperature and melt fraction distributions.

Velocity of a wave through any material is calculated using the seismic wave equation, based on stress and strain theory. The three parameters which affect p-wave and s-wave velocity in a homogeneous, isotropic, solid medium are the shear modulus, μ , the bulk modulus, K , and the density, ρ , as shown in equations 4.1 and 4.2.

$$v_p = \sqrt{\frac{K + \frac{4}{3}\mu}{\rho}} \quad (4.1)$$

$$v_s = \sqrt{\frac{\mu}{\rho}} \quad (4.2)$$

All three dependent variables in the wave equation; density, bulk modulus, and shear modulus, can be shown to be dependent on both melt fraction and temperature (Birch, 1961). Thus, variations in the lateral and vertical distribution of temperature and melt in the crust result in observed seismic velocities that depart from the expected background crustal velocity gradient such as that calculated in the Preliminary Reference Earth Model (PREM) (Dziewonski and Anderson, 1981).

Before the velocity anomaly attributed to either temperature or melt fraction can be determined, the elastic moduli have to be estimated. The two elastic moduli that we concern ourselves with in this thesis are the bulk and shear moduli. The bulk modulus of a rock is its relative change in volume caused by uniform application of compressive, or tensile, stress. Shear modulus is also termed the shear stiffness of a rock and is the ratio of shear stress to shear strain.

Dependence of seismic velocity on temperature is derived from both anharmonic (frequency-independent) and anelastic (frequency-dependent) mechanisms (Karato, 1993). The anharmonic component of the dependence of seismic velocity on temperature is derived from the change in the shear modulus associated with a variation in temperature. There is an inverse relationship between temperature heterogeneity and seismic velocity, with low temperature regions having high velocities and vice versa (Karato and Karki, 2001). This is due to the effect that temperature of a medium has on its density and elastic moduli through thermal expansion. Despite having a low average coefficient of thermal expansion, the crystalline nature of the crust results in measurable, and significant, velocity anomalies in regions where the temperature departs from the expected background crustal temperature. As temperature increases the rigidity of the rocks in the crust reduces, thereby lowering the velocity at which seismic waves are able to travel through the region. The anelastic component of the dependence of seismic velocity on temperature is due to frequency-dependent visco-elastic relaxation in the medium through which the wave travels. While the inverse relationship between temperature variation and seismic velocity is apparent in both the crust and the mantle, it is more complex in the shallow crust due to the dominant influence of porosity and compositional heterogeneities (Paulatto et al., 2012).

The presence of melt in the crust and its contribution to vertical and lateral velocity anomalies must be dealt with separately from the effect of temperature to simplify the problem and avoid over-estimation of the anomaly. While the effects of temperature and melt fraction could be dealt with together this would require knowledge about the phase diagram of the melt which is not always available. The sensitivity of a medium's elastic moduli to the presence of fluid directly correlates with the effect of fluid saturation on velocity through the medium (Han and Batzle, 2004). Gassmann's equations for the dependence of velocity on fluid fraction are valid in domains where pore-pressure is in equilibrium as is assumed to be the case in the thermo-mechanical model (Eberhart-Phillips et al., 1989; Batzle et al., 2006). As such, Gassmann's equation provides a method of determining the additional contribution from the presence of melt to the overall velocity anomaly in the domain.

For the purposes of this thesis partially molten rocks, representing a crystal-rich mush, will be treated as a multi-phase material. There are a number of possible approaches for calculating the elastic properties of composite, multiphase materials including adoption of scattering theory, use of variational principles, and assuming pre-defined geometries for the constituents of the composite medium in question (Watt et al., 1976). The various approaches differ in their results in terms of mathematical categorisation, with the possibility of determining elastic moduli in the form of upper and lower bounds, single estimates, and exact results for any particular composite (Berryman, 1995). Effective medium

estimates can be categorised as either implicit or explicit methods (Kuster and Toksöz, 1974a,b; Berryman, 1980a; Norris, 1989). While explicit schemes provide expressions that can be easily applied and inverted, implicit methods need to be solved by iteration (in the case of the self consistent method) or by integration. The increased stability of implicit schemes in comparison with explicit schemes makes them extremely useful, particularly in cases where large time steps are required.

The large number of potential methods available for calculating the effective elastic properties of a heterogeneous composite medium arose from the need in the mid 20th century for composite materials with specific properties for use in engineering (Watt et al., 1976). As a result, although a wide variety of methods exists, many of them are applicable only to very specific cases and only a few are applicable more generally. Effective medium theory was originally developed for application in the field of dielectrics in composite media by Bruggeman (1935) but has since been applied to geological studies (Bergman, 1978).

Due to their inherently heterogeneous nature, rocks present a complex problem when attempting to determine their elastic properties. The various mineralogical components of rocks are anisotropic and can have very different compositional and elastic properties. In addition, the variation in grain sizes not only between different rock types but also between the minerals found in rocks results in heterogeneity of elastic properties on a number of length scales (Watt et al., 1976). For the estimation of the elastic moduli carried out in this thesis the effect of variation in grain size is assumed to be negligible due to the large wavelengths of surface seismic data. The problems laid out in this work were further simplified by assuming the effect of anisotropy to also be negligible.

For the composites studied in this thesis it is most practical to look at initially defining upper and lower bounds on the elastic moduli due to the inherent uncertainty in the constraints on parameters associated with melt segregation and crustal properties. Various bounds have been determined for the physical constants of heterogeneous composites based on variational principles and criteria for thermodynamic stability (Berryman and Milton, 1991).

The best known bounds for elastic moduli are the Voigt (upper) and Reuss (lower) variational bounds (Man and Huang, 2011). The Voigt bound described by Voigt (1928) is often referred to as the rule of mixtures, as it takes a volume average of the different constants attributed to the component parts of a heterogeneous composite. It is calculated under the assumption that strain is uniform throughout the composite in question. The equation for the Voigt bound for the bulk modulus, K_v , is shown in equation 4.3, and the shear modulus, μ_v , is shown in equation 4.4. In contrast, the Reuss bound, as

described by Reuss (1929) is a harmonic mean of the constituent physical constants of a heterogeneous composite. The Reuss bound assumes constant stress throughout the entire medium and therefore represents the case of a fluid suspension. The equation for the Reuss bound on the bulk modulus, K_r , is shown in equation 4.5, and the Reuss bound for the shear modulus, μ_r , is given in equation 4.6. It can be seen from the equations that both bounds use a weighted average for the constituents where f_i describes the volume fraction of the i^{th} constituent.

$$K_v = \sum_{i=1}^{i=n} f_i K_i \quad (4.3)$$

$$\mu_v = \sum_{i=1}^{i=n} f_i \mu_i \quad (4.4)$$

$$K_r^{-1} = \sum_{i=1}^{i=n} f_i K_i^{-1} \quad (4.5)$$

$$\mu_r^{-1} = \sum_{i=1}^{i=n} f_i \mu_i^{-1} \quad (4.6)$$

Due to the nature of these two means, they provide upper and lower estimates for the effective elastic moduli of a medium. Hill (1952) used variational principles to prove the rigour of these two bounds for elastic constants and later produced a self-consistent approach which produced an estimate that was also shown to fall between the two bounds (Hill, 1965). In the case where a single estimate of the true value is required for the elastic moduli, the Voigt-Reuss-Hill (VRH) average is often taken as the average of the Voigt and Reuss bounds as shown in equation 4.7, where either the bulk or shear moduli can be substituted for M .

$$M_h = \frac{M_v + M_r}{2} \quad (4.7)$$

It is possible to provide stricter bounds on the elastic moduli of a composite than the Voigt and Reuss bounds but only when the volume fractions of the constituents are known. The Hashin-Shtrikman bounds, calculated using variational principles in elastic theory, have been shown to fall within the Voigt and Reuss bounds (Hashin and Shtrikman, 1962). The VRH average has also been shown to lie within the Hashin-Shtrikman bounds in nearly all cases except where the fluid fraction nears unity (Watt, 1980).

Hashin-Shtrikman bounds apply to quasi-homogeneous and quasi-isotropic multiphase materials (Hashin and Shtrikman, 1963). A general form of the bounds was found by (Berryman and Berge, 1993) to be applicable in the case of two or more phases being mixed. Equation 4.8 and equation 4.9 give the upper and lower Hashin-Shtrikman bounds respectively for the bulk modulus, K . The upper and lower bounds for the shear modulus can be calculated using equations 4.10 and 4.11. The indices μ, K_f and μ, K_s refer to the moduli for the fluid and solid phases respectively and the melt fraction is represented by ϕ .

$$K_{HS}^+ = K_s + \frac{\phi}{(K_f - K_s)^{-1} + (1 - \phi)(K_s + \frac{4}{3}\mu_s)^{-1}} \quad (4.8)$$

$$K_{HS}^- = K_f + \frac{\phi}{(K_s - K_f)^{-1} + (1 - \phi)(K_f + \frac{4}{3}\mu_f)^{-1}} \quad (4.9)$$

$$\mu_{HS}^+ = \mu_s + \frac{\phi}{(\mu_f - \mu_s)^{-1} + \frac{2(1-\phi)(K_s + 2\mu_s)}{5\mu_s(K_s + \frac{4}{3}\mu_s)}} \quad (4.10)$$

$$\mu_{HS}^- = \mu_f + \frac{\phi}{(\mu_s - \mu_f)^{-1} + \frac{2(1-\phi)(K_f + 2\mu_f)}{5\mu_f(K_f + \frac{4}{3}\mu_f)}} \quad (4.11)$$

Another set of bounds have been determined using an explicit scheme by Kuster and Toksöz (1974a,b) which can be shown to be identical to the Hashin-Shtrikman bounds for the case of spherical inclusions and long wavelengths (Kuster and Toksöz, 1974a,b; Berryman, 1980a). The Kuster-Toksöz method

replaces the composite medium for which elastic constants are being estimated with a large sphere containing inclusions, as shown in figure 4.1. The matrix and the inclusions in the sphere are given distinct compositional properties. Kuster and Toksöz (1974a) performed hypothetical experiments to determine the scattering within a large sphere caused by the smaller spherical inclusions. It was found that the total amount of scattering from the inclusions depended on their total volume concentration (Kuster and Toksöz, 1974a; Berryman, 1980a).

The Kuster-Toksöz effective elastic moduli however are only valid at low inclusion concentrations, i.e. low melt fractions because they ignore interactions between adjacent pore spaces (Berryman, 1980a). In the case of low inclusion concentration, the total scattering is equivalent to that which would occur in a homogeneous large sphere with the same effective elastic constants as the composite sphere containing the matrix and inclusions of two different rock types (Kuster and Toksöz, 1974a). The method is limited in its usefulness for the thermo-mechanical modelling presented in this thesis due to the high melt fraction sills that are input into the system and the melt layers that accumulate over time via melt segregation.

This thesis uses a self-consistent scheme modified by Berryman (1980a, 1995, 2005), which in itself uses checks on the bounds of the elastic moduli following the methods of Hashin and Shtrikman (1962, 1963) and Hill (1963). Berryman's approach to the self-consistent method is symmetric in that none of the constituents making up the multi-phase material are treated preferentially. Rather, the liquid-filled pores and the solid grains must be added to the effective background in the correct proportions. As such, Berryman's method is superior to other potential self-consistent schemes that could be used such as the approach of Schmeling (1985). The method has been tested computationally by Berryman (1995) and stress-tested under various conditions. Results of the tests provide convincing evidence that the method is consistent with the most rigorous bounds on elastic moduli known for inhomogeneous materials and therefore a viable method for use in this thesis (Berryman, 1995, 2005).

The mixture theory described by Berryman (1995) can only be used if the mineral content and relative volume fractions of each constituent of the heterogeneous composite are known. This is the case for the thermo-mechanical model used in this work as the petrological parameters are defined by the user and are specified for the different rock types used. The main difference between the self-consistent method of Berryman (1995) and that of Kuster and Toksöz (1974a,b) can be seen schematically by comparing the structures of the modelled composites in figures 4.1 and 4.2.

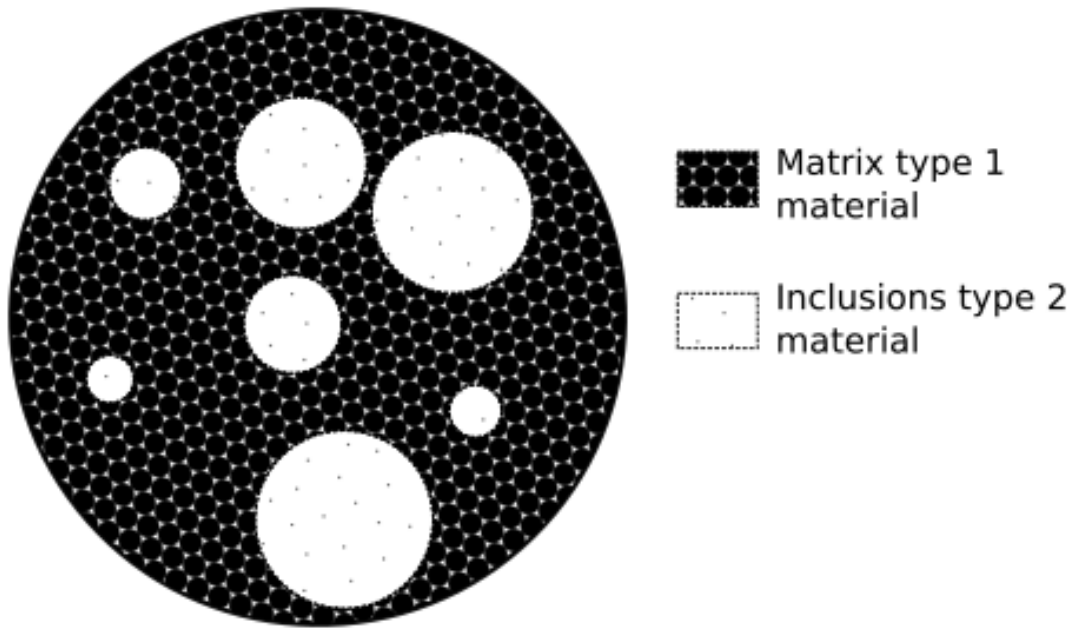


Figure 4.1: Adapted from Berryman (1980a). Schematic diagram of the composite used in the Kuster-Toksöz explicit estimation of the effective elastic moduli of a composite medium. The true composition of the heterogeneous composite is replaced in this instance by the large circle which denotes the matrix of rock type 1 and within which inclusions of rock type 2 are found. Drawing is not to scale.

Mixture theory, as applied specifically to rocks, can produce both bounds and estimates on the elastic constants for a composite rock (Berryman, 1995). In cases which include porosity, as in the thermo-mechanical model, studies have generally gravitated toward the use of estimates rather than bounding methods (Berryman, 1980a). Bounds are able to provide useful estimates for polycrystalline materials due to the small variations in the elastic moduli of the various constituents. However, due to the effect that porosity has in bringing one of the bounds either to infinity or to zero in multi-phase media, the calculated bounds end up being so far apart that they do not provide a useful range and so single estimates are preferred (Berryman, 1980a).

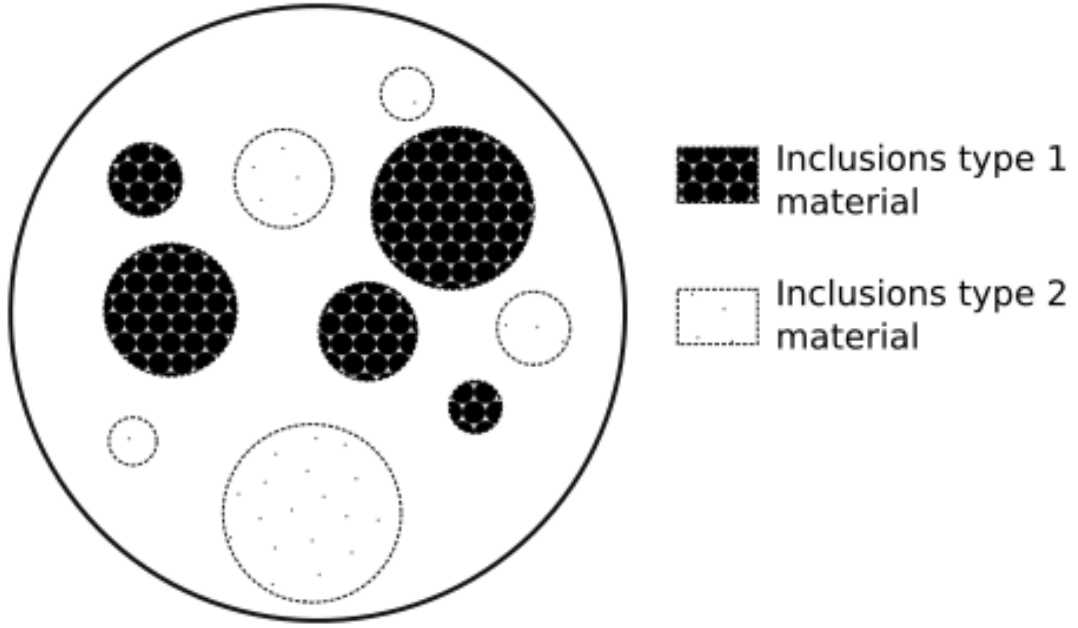


Figure 4.2: Adapted from Berryman (1980a). Schematic diagram of the composite used in the Berryman self-consistent estimation of the effective elastic moduli of a composite medium. The true composition of the heterogeneous composite is replaced in this instance by the large circle which contains inclusions of both rock type 1 and 2. Drawing is not to scale.

4.2 Method

The estimates for the bulk and shear moduli were calculated using an iterative numerical model based on the original results from the 1D thermo-mechanical model for temperature and melt fraction. Initially, a background velocity profile was created across the entire 2D section, including a sea depth of 1km at the top of the profile and a flat bathymetry for the sea floor. The P-wave velocity in the sea water was set to be constant at $\nu_w = 1.50\text{kms}^{-1}$. The velocity gradient of the crust between the surface and the depth of the Moho was set to vary between $\nu_c = 3.50\text{kms}^{-1}$ and $\nu_c = 7.50\text{kms}^{-1}$ based on average values from PREM and studies of upper crustal seismic velocities (Dziewonski and Anderson, 1981; Christensen and Mooney, 1995; Dunn et al., 2000). The P-wave velocity gradient across the Moho and upper mantle were set to be 1.00 and 0.08 km s^{-1} respectively. These deeper

values are essentially nominal due to the shallow nature of the models which do not reach the average depth of the continental Moho as determined by Cook (2002).

Karato's method was then used to determine the contribution of temperature variations along the 1D profile to the calculated seismic anomaly (Karato, 1993). As can be seen in equation 4.14, the derivative of $\ln(v_p)$ with respect to temperature depends on temperature itself and as such has been solved iteratively. The iterative approach involves continuously updating the velocity anomaly over a large number of increments until the least squares difference between two successive values was determined to be sufficiently small (on the order of 10^{-4}). Once the elastic moduli and P-wave velocities were calculated they were then extrapolated laterally to give an estimated 2D velocity profile.

Temperature derivatives of both P-wave velocity and density have been determined by many studies to be due mostly to anharmonic effects (Kumazawa and Anderson, 1969; Isaak, 1992; Karato, 1993). In the case of the model domain used in this thesis, anharmonicity can be defined as a departure from the assumption that the specific heat capacity, thermal expansion coefficient, and pressure-dependent bulk modulus are independent of temperature variations when volume is kept constant (Stacey and Isaak, 2003). Thermal expansion and the pressure dependence of a material's bulk modulus are considered to be first-order anharmonic effects, while temperature dependence of a material's specific heat capacity and the product of bulk modulus and the thermal expansion coefficient are higher-order anharmonic effects (Karato and Karki, 2001; Stacey and Isaak, 2003).

While anharmonicity has been determined to have a large effect on the temperature dependence of P-wave velocity, the studies by Kumazawa and Anderson (1969) and Isaak (1992) were conducted at high frequencies of approximately 1MHz while seismic surveys are conducted at frequencies <1 MHz. P-wave velocity at these lower frequencies depends more strongly on anelastic effects caused by temperature variations (Karato, 1993). In addition, it has been shown that anharmonic effects alone are too small to account for observed seismic velocity anomalies due to temperature and cannot explain the low velocity heterogeneity ratio between shear to compressional waves observed (Karato and Karki, 2001).

Anelastic effects therefore also had to be taken into account when calculating the contribution of temperature variations in the modelled domain to the predicted seismic velocity anomaly but are secondary to the effects of anharmonicity in this study. This is because anelasticity is most important when considering the effect of temperature on shear wave velocity and only the P-wave, or compressional wave, velocity was estimated to produce a P-wave velocity profile. In addition, anharmonic

effects have been shown to decrease with increasing pressure and so dominate in the upper crust but decrease through the mantle, making anharmonic effects more significant in shallow crustal modelling (Chopelas and Boehler, 1989, 1992; Chopelas, 1992). It has been shown that when both the anelastic and anharmonic effects are considered while determining the thermal dependence of seismic velocity in the crust, the majority of an observed velocity anomaly can be accounted for (Karato and Karki, 2001). The remaining anomaly in geophysical observations must then be accounted for through compositional heterogeneity and structural anisotropy. Due to the synthetic nature of the problem in this thesis lateral compositional heterogeneity in the modelled profile can be ruled out. As a result, the method of Karato (1993) was determined to be sufficient for use in this thesis to calculate only the thermal contribution to the seismic P-wave velocity anomaly.

The P-wave velocity, ν , at any particular point can be calculated using equation 4.12 (Kanamori and Anderson, 1977; Karato and Spetzler, 1990; Karato, 1993). T is the temperature, ν_0 is the background velocity (as calculated using the velocity gradient method described above), ω is the frequency, and τ is a temperature-dependent relaxation time (Karato, 1993). In this instance the attenuation, Q , is set at 200 and is assumed to be independent of frequency (Paulatto et al., 2010).

$$\nu = \nu_0(T) \cdot \left(1 + \left(\frac{Q^{-1}}{\pi}\right) \ln \omega \tau(T)\right) \quad (4.12)$$

The relaxation time, τ is determined by equation 4.13, where τ_0 is a set factor, R is the gas constant (8.314), and H_a is the activation enthalpy of the system, set to be $2.76 \times 10^5 \text{ kJmol}^{-1}$ (Caristan, 1982).

$$\tau = \tau_0 \exp\left(\frac{H_a}{RT}\right) \quad (4.13)$$

Finally, the velocity anomaly due to thermal inhomogeneity is found by taking the partial temperature derivative of equation 4.12 as is shown in equation 4.14. The anharmonic effects are described by the first term in equation 4.14, while the second term in the equation describes the temperature contribution from anelastic and viscoelastic effects (Karato, 1993). $F(\kappa)$ is a factor that describes the exponential dependence of attenuation, or the quality factor, Q , on frequency.

$$\frac{\partial \ln \nu}{\partial T} = \frac{\partial \ln \nu_0}{\partial T} - F(\kappa) \cdot \frac{Q^{-1}}{\pi} \frac{H_a}{RT^2} \quad (4.14)$$

Equation 4.14 was solved iteratively, following the technique used by Paulatto et al. (2012). The anharmonic term was assumed to be constant at $-8.5 \times 10^{-1} K^{-1}$ (Christensen, 1974). The anelastic part of equation 4.14 was calculated by assuming that $F(\kappa) = 1$, equivalent to there being no dependence on frequency (Paulatto et al., 2012). The velocity anomaly attributable to temperature variations was then added to the background velocity profile for the sill-emplacement region where the 1D thermo-mechanical solution for temperature and melt fraction distribution had been calculated. This gave a 1D P-wave velocity solution for the solid matrix in the thermo-mechanical model.

The S-wave velocity was then calculated from the P-wave velocity using an empirical relation determined by Brocher (2005). Brocher (2005) determined S-wave velocity as a function of P-wave velocity for a range of common lithologies from various field sources using simple linear regression. The relationship used in this thesis is shown in equation 4.15, and is referred to as 'Brocher's regression fit' in Brocher (2005). Equation 4.15 is valid between 1.5 and 8.0 kms^{-1} with a calculated coefficient of determination, R^2 , of 0.979 (Brocher, 2005). This forms the basis for the highest value for P-wave velocity used in the background 2D velocity profile at depths shallower than the Moho discontinuity. Velocities in Brocher's regression fit are input in units of kms^{-1} .

$$V_s = 0.7858 - 1.2344V_p + 0.7949V_p^2 - 0.1238V_p^3 + 0.0064V_p^4 \quad (4.15)$$

Initial values for the bulk and shear moduli of the partially molten region were then calculated along the 1D profile from the V_p , V_s , and matrix density (ρ_s) values. The initial matrix bulk modulus, K_{s0} was calculated using equation 4.16, and the initial matrix shear modulus, μ_{s0} using equation 4.17. Both equations 4.16 and 4.17 can be derived from equation 4.1 for P-wave velocity.

$$K_{s0} = \rho_c(V_p^2 - \frac{4}{3}V_s^2) \quad (4.16)$$

$$\mu_{s0} = \rho_c V_s^2 \quad (4.17)$$

Melt geometry is an important consideration in this approach however it is poorly constrained for melt accumulation during repetitive sill emplacement in the crust (Berryman, 1980a; Paulatto et al., 2012).

The most significant differences in seismic velocity due to geometry occur according to whether pockets of melt are assumed to be isolated or interconnected within the medium (Berryman, 1980a).

The self-consistent approach considers each individual pocket of melt as being embedded within a homogeneous material which is assumed as having the elastic properties of the composite medium being determined (Berryman, 1980a). Each constituent within the medium is therefore treated in the same manner, rather than separating the calculations out for the matrix and the melt phases. This makes the two phases essentially interchangeable within the equations and results in the self-consistent approach being valid even at very high melt fractions (Paulatto et al., 2012). This is useful for the cases studied in this thesis where melt segregation occurs and melt is able to accumulate very quickly into high melt fraction layers.

It has been shown that melt pocket shape is directly correlated with melt fraction such that the melt pocket shape evolves through time as melt fractions change (Smith, 1964). Melt begins to form in tubular shaped pockets along grain edges and in pore spaces during melting at low melt fractions (Smith, 1964; Waff and Bulau, 1979; Mavko, 1980). As melt accumulates or as temperatures rise and melt fraction increases the distance between grains increases and the geometry of the melt resembles wider pipes (Waff and Bulau, 1979). In order to capture this behaviour in the modelling, the aspect ratio, A , of the melt pockets was set to be dependent on the melt fraction, ϕ , using the method of Kiddle (2011) as can be seen in equation 4.18. This results in spheroidal melt pockets which are oblate when equation 4.18 is >1 and prolate when equation 4.18 is <1 .

$$A = \frac{1}{2} \cdot \frac{1}{\sqrt{\phi}} \quad (4.18)$$

The seismic velocity anomaly in a medium containing melt pockets is also significantly affected by velocity dispersion mechanisms which occur due to the presence of the fluid, such as the flow of melt along grain boundaries and between interconnected pore spaces (Annen et al., 2014). Elastic moduli, and therefore seismic velocities, are dependent on frequency. While ideally it would be possible to calculate the full frequency-dependent values for the elastic moduli of a medium this is rarely possible due to the complexity of the problem. As such, the moduli are estimated in the limits of infinitely low and infinitely high velocities (Kiddle, 2011). It has been shown by Budiansky and O'Connell

(1976) that for low seismic velocities, flow between interconnected pockets of melt equalises pressure imbalances caused by the passing wave and dissipates energy. This is referred to as a low-frequency approximation to the solution for the velocity anomaly, corresponding to a long wavelength of the incident plane-wave travelling through the medium. In contrast, the high-frequency approximation occurs when melt pockets are not interconnected and melt is not able to flow between the pore spaces and accumulate (Budiansky and O’Connell, 1976; O’Connell and Budiansky, 1977). The low-frequency approximation leads to reduced values for seismic wave velocities and larger negative velocity anomalies than the high-frequency approximation. The microscopic processes that cause dispersion (frequency dependence) have relaxation frequencies that are mostly higher than the seismic band (0.1 - 10 Hz), therefore the low-frequency approximation is more appropriate (Kiddle, 2011).

In the case of the high-frequency approximation, the initial bulk modulus of the melt, K_{m0} , was set to be 12.7 MPa, consistent with the work of Paulatto et al. (2012) and the studies on silicic melt by Rivers and Carmichael (1987). For cases where the low-frequency approximation was used, the initial bulk modulus of the melt was set to a nominal value of 0.1 MPa. This value was chosen by attempting to minimise the mis-fit between the results found by this work and that of Paulatto et al. (2012) shown in figure 4.4 for the relationship found at constant temperature between seismic velocity and melt fraction. The initial shear modulus of the melt, μ_{m0} , in both the high-frequency and low-frequency approximations was set to be 0 MPa.

Effective density values were set in regions where the melt fraction, ϕ was >0 using the calculation shown in equation 4.19. This was done to ensure that the densities used to calculate the final elastic moduli through Berryman’s iterative method were consistent with the homogeneous medium approach.

$$\rho_{eff} = \rho_{melt}\phi + \rho_{solid}(1 - \phi) \quad (4.19)$$

The velocity anomaly corresponding to the presence of melt in the 1D section was then calculated and added to the background velocity of the profile. This was done by initially calculating the Voigt (upper) and Reuss (lower) variational bounds and the Hill average for the bulk and shear moduli of the composite medium as an initial guess for the iterative approach of Berryman (1980a). Equations 4.3 - 4.7 were used, with the melt and the solid fractions used respectively as the constituents f_m and f_s .

The Hill averages for both the shear and bulk moduli were then used as initial estimates for the true shear and bulk moduli of the composite medium in an iterative solver. The method uses a least-squares convergence between the values for the bulk and shear moduli calculated using Berryman's self-consistent method and the bulk and shear moduli initially set using the Hill average. On each successive iteration the initial values were updated until convergence was reached.

The self-consistent method described by Berryman (1980a,b, 1985, 1995, 2005) that was adapted for use in this thesis provides options for determining the effective elastic moduli of a heterogeneous material for a number of different inclusion geometries. The original study carried out in 1980 outlined the new approach to calculating effective elastic moduli and was used for the simple case of spherical inclusions. Further studies applied the same method to various cases of ellipsoidal inclusions, each with different aspect ratios, as well as to polycrystals. Spherical and ellipsoidal approaches were also used by Paulatto et al. (2012) and Annen et al. (2014) to determine a possible range of melt fractions from travel-time tomography data. In order to be able to make a direct comparison with these previous results, which are purely thermal and assume a linear relationship between melt fraction and temperature, the conversion from temperature and melt fraction values to seismic P-wave velocity values developed for this thesis also allowed for a number of melt geometries to be used.

The geometry-specific calculations followed the self-consistent approach of Berryman (1980a,b) and were implemented using the method of Paulatto et al. (2012). Melt pocket geometries were specified at the start of the conversion process by user-inputted values and the relevant calculations were then carried out within the iterations. Four options for melt pocket geometry were calculated, as described in table 4.1, in order to be comparable with those calculated by Paulatto et al. (2012). The coefficients P and Q are defined in equations 4.20 and 4.21 respectively, where T is a tensor which relates two static strains for the case of spherical inclusions, as defined by Te Wu (1966) in equation 4.22. ϵ_{PQ} is the strain field within the inclusions in the multiphase medium, and ϵ_{PQ}^0 is the uniform strain at infinity (Te Wu, 1966; Berryman, 1980b).

$$P = \frac{1}{3}T_{PPQQ} \quad (4.20)$$

$$P = \frac{1}{5}(T_{PQPQ} - P) \quad (4.21)$$

$$T_{PQRS} = \frac{\epsilon_{PQ}}{\epsilon_{RS}^0} \quad (4.22)$$

Berryman (1980a) was used to determine the impact of spherical inclusions on the relationship between P-wave velocity and melt fraction. The three further options in table 4.1 were all based on the parameters provided in table 1 of Berryman (1980b) which considers the cases of prolate and oblate spheroidal inclusions as well as that of melt-dependent variable aspect ratio. Spheroidal inclusion geometries are in essence simply a more general case of the spherical melt pocket geometries. The cases of prolate and oblate spheroids, referred to by Berryman (1980b) as 'needles' and 'disks', were originally derived by Te Wu (1966). Derivation of the case for spheroids with variable aspect ratio, referred to by Berryman (1980b) as 'penny-shaped cracks', was first carried out by Walsh (1969). This case can be seen to be dependent on the aspect ratio, α .

Inclusion Shape	P	Q
Spheres	$\frac{K_m + \frac{4}{3}\mu_m}{K_i + \frac{4}{3}\mu_m}$	$\frac{\mu_m + F_m}{\mu_i + F_m}$
Needles	$\frac{K_m + \mu_m + \frac{1}{3}\mu_i}{K_i + \mu_m + \frac{1}{3}\mu_i}$	$\frac{1}{5} \left(\frac{4\mu_m}{\mu_m + \mu_i} + 2 \frac{\mu_m + \gamma_m}{\mu_i + \gamma_m} + \frac{K_i + \frac{4}{3}\mu_m}{K_i + \mu_m + \frac{1}{3}\mu_i} \right)$
Disks	$\frac{K_m + \frac{4}{3}\mu_i}{K_i + \frac{4}{3}\mu_i}$	$\frac{\mu_m + F_i}{\mu_i + F_i}$
Penny-shaped cracks	$\frac{K_m + \frac{4}{3}\mu_i}{K_i + \frac{4}{3}\mu_i + \pi\alpha\beta_m}$	$\frac{1}{5} \left(1 + \frac{8\mu_m}{4\mu_i + \pi\alpha(\mu_m + 2\beta_m)} + 2 \frac{K_i + \frac{2}{3}\mu_i + \frac{2}{3}\mu_m}{K_i + \frac{4}{3}\mu_i + \pi\alpha\beta_m} \right)$

Table 4.1: Taken from Berryman (1980b). The subscripts m and i refer to the matrix and the inclusions respectively. The characters F, γ , and β are defined as: $F = \frac{\mu}{6} \frac{9K+8\mu}{K+2\mu}$, $\gamma = \mu \frac{3K+\mu}{3K+7\mu}$, and $\beta = \mu \frac{3K+\mu}{3K+4\mu}$

The coefficients determined using table 4.1 are then used in the implicit equations 4.23 and 4.24 to determine the bulk (K) and shear (μ) moduli respectively. These two equations form the iterative self-consistent scheme as set out by Berryman (1980b). P and Q are as set out in table 4.1, while c is the elastic tensor of the multiphase medium and the star denotes the parameters for the background matrix of the medium.

$$(K^*)_{n+1} = \frac{\sum_{i=1}^N c_i K_i (P^{*i})_n}{\sum_{i=1}^N c_i (P^{*i})_n} \quad (4.23)$$

$$(\mu^*)_{n+1} = \frac{\sum_{i=1}^N c_i \mu_i (Q^{*i})_n}{\sum_{i=1}^N c_i (Q^{*i})_n} \quad (4.24)$$

Finally, Gassmann's equation for fluid substitution was used to include the effects of filling the pore spaces with melt for the low-frequency case of interconnected melt pockets (Gassmann, 1951a,b; Smith et al., 2003). This is an important step when considering the low-frequency case and requires first removing the effect of the melt found in the previous calculations. The method of Berryman (1980a), if used on its own, gives a result only for the high-frequency approximation (unrelaxed modulus). To get the low-frequency approximation (relaxed modulus) the modulus of the dry matrix was first calculated by setting the bulk modulus of the fluid to essentially 0, and Gassmann's equation was used to perform the fluid substitution. Gassmann's equation relates the bulk modulus of the matrix when saturated with melt to the elastic properties of both the matrix and the melt alone (Smith et al., 2003). It is only valid for the low-frequency approximation as the equation assumes not only that the medium is homogeneous and isotropic, but also that the pore spaces are completely interconnected (Gassmann, 1951a; Smith et al., 2003).

Gassmann's equation does not take into consideration the geometry of the pore spaces and is therefore a relatively simple assumption to implement, as can be seen by equations 4.25 - 4.26. Despite its simplicity, this approach has been shown to be incredibly accurate (Mavko et al., 2009; Misaghi et al., 2010). The equations assume that the melt phase is homogeneously distributed throughout the pore spaces in the modelled medium. This is a valid assumption to make for cases where modelling occurs over geologic time as the system will come to equilibrium and the melt will become evenly distributed.

Implementing Gassmann's equation only affects the final value of the bulk modulus for the composite medium in the low-frequency approximation. This is because the bulk modulus may vary according to the composition of melt in the pore spaces whereas the shear modulus is insensitive to pore fluid composition as it is by definition zero for a fluid (Smith et al., 2003). As a result, the shear modulus is left unchanged after applying Gassmann's equation for fluid substitution.

$$K_{saturated} = \frac{K_{s0}(K_s + f_0)}{K_{s0} + f_0} \quad (4.25)$$

$$f_0 = \frac{K_{m0} \frac{(K_{s0} - K_s)}{\phi}}{K_{s0} - K_{m0}} \quad (4.26)$$

Final p-wave velocity values were then calculated for each grid cell in the 1D domain from the estimates for the corresponding elastic moduli. This was done using equation 4.1, with the effective density, ρ_{eff} , calculated in equation 4.19 substituted for ρ .

Once all of the velocity values had been calculated for the 1D section, the 2D velocity profile was calculated. The 1D section was repeated across the width of the sill emplacement zone. As a result, the 2D profile does not account for the lateral movement of melt or temperature within the sill emplacement zone.

A linear geothermal gradient was used to determine the background temperature of the crust for the thermo-mechanical model. The 1D temperature outputs were then used to calculate the lateral diffusion distance of heat outwards from the edge of the sills in the profile over the total run time of the model from the first sill emplacement. This was done individually at each node in the temperature profile using equation 4.27, taken from Carslaw and Jaeger (1959). D is the non-dimensional characteristic diffusion distance within the model (expressed as a number of grid nodes), κ is the thermal conductivity of the country rock into which heat is diffusing, ρ_c is the density of the country rock, C_p is the specific heat capacity, L_f is the latent heat of fusion (or enthalpy of crystallisation), τ is the time (in seconds) over which temperature perturbation occurred, δT is the temperature difference between the sill and the background geotherm, and δx is the width (in metres) of a single grid cell. A discussion of the use of equation 4.27 can be found in the Appendix to this thesis.

$$D = \frac{\sqrt{\tau \cdot \frac{\kappa}{\rho_c \cdot (C_p + \frac{L_f}{\delta T})}}}{\delta x} \quad (4.27)$$

The diffusion distance was then used as the basis for a bi-linear interpolation of P-wave velocity values from the edge of the sill emplacement zone into the surrounding country rock. Due to the perturbation of the geotherm by the influx of melt, the calculated diffusion distances were largest in the sill emplacement zone and decreased with distance from the emplacement zone until the background temperature profile was reached. The interpolation was assumed to be symmetrical either side of the central axis of the emplacement zone.

Results from the thermo-mechanical model were modified to reduce the total domain depth in 1D and thereby make the final 2D velocity profile more manageable for post-processing. This was possible partly due to the nature in which new sills are brought in to the thermo-mechanical model, by shifting down the domain below the emplacement depth by the thickness of the new sill and thereby incrementally increasing the domain size, resulting in extra cells at the base of the system.

4.3 Results

A number of tests were carried out on the method outlined above to ensure that it was valid in the situations for which it was used. In addition, the results were benchmarked against the work of Paulatto et al. (2012) to ensure that the estimations for P-wave velocity found using the code developed by the author for this work are able to match those of previous studies. In all three tests carried out and displayed in figures 4.3 - 4.5, the temperature was kept constant and only the melt fraction was varied. This was done to test the implementation of Berryman's self-consistent method for the effect of melt fraction on seismic velocity used in this thesis.

The high-frequency approximation to the P-wave velocity solution was tested to ensure that the calculation of the bounds for the elastic moduli matched those found by Paulatto et al. (2012) across the full range of possible melt fractions from $\phi = 0$ to $\phi = 1$. The results are shown in figure 4.3 which plots the final P-wave velocity value against melt fraction.

The dashed lines in figures 4.3 and 4.4 represent the velocity solution determined by the author for this thesis while the solid lines show the solution presented by Paulatto et al. (2012). The two solutions match perfectly for the case where the Hashin-Shtrikman upper and lower bounds for the elastic moduli were used to determine upper and lower bounds to the velocity solution. Figures 4.3 and 4.4 show a slight discrepancy in the results using both the high-frequency and low-frequency approximations when different melt geometries are considered and the iterative method of Berryman (1980a) is used to solve for the elastic moduli, with the Hill averages for the bulk and shear moduli taken as the initial values for use in the calculations.

The differences between Paulatto et al. (2012) and the results in this thesis can be explained by the use of different initial parameters in the two solutions. The temperature at which the melt-velocity relationships are calculated by Paulatto et al. (2012) is not given but has been assumed to be the solidus value of andesite (approximately 700°C). In addition, the convergence criterion in Paulatto

et al. (2012) for the least squares of the elastic moduli, at which the iterations are stopped and the velocity is calculated, is not known. This could affect the results due to the possibility of either of the solutions not reaching adequately small convergence criteria.

The main difference between the two melt-velocity relationships most likely arises from differences in the calculation of aspect ratio for the various melt pocket geometries tested. Paulatto et al. (2012) investigate four different melt pocket geometries; spheres, oblate spheroids, prolate spheroids, and spheroids whose aspect ratio is dependent on melt fraction. These four cases relate to the geometries studied by Berryman (1980a) and Berryman (1980b).

The estimation in this work of seismic velocity using prolate spheroidal melt pocket geometry can be seen in figure 4.3 to deviate furthest from the estimation (up to 4%) carried out by Paulatto et al. (2012) when the high-frequency approximation is used. In contrast, the low-frequency approximation results in figure 4.4 show the greatest deviations (up to 6%) in the cases of variable aspect ratio and oblate spheroids.

In the low-frequency case, the difference in shape between the two sets of results is most likely to be associated with the initial values used for the bulk and shear moduli of the melt phase when starting the iterative calculations of the self-consistent method. The initial bulk modulus chosen for use in this work was set at 0.1 MPa. The value was determined by trying to minimise the misfit seen between the results of Paulatto et al. (2012) and those found in this thesis for all four different options of melt pocket geometries. For the high-frequency case, the discrepancy is most likely to be due to a difference in the final calculations used to determine the exact aspect ratio for the prolate spheroids as well as the exact relationship used for the case of melt fraction dependent variable aspect ratio. Therefore, the overall match between the two models shown in figures 4.3 and 4.4 was deemed to be acceptable.

Figure 4.5 shows the results of a convergence test for the least-squares difference in the elastic moduli calculations. The graph shows the results for the dependence of seismic velocity on melt fraction at constant temperature. The value for the least-squares difference at which convergence was said to have been attained was decreased by a factor of 10 from 1000 to 0.1Pa successively. This effectively reduces the value which was considered as an acceptable difference between the values of the iteratively updated moduli between two successive time steps. The smaller the difference, the closer the moduli are to converging on a constant value. As a result, it is expected that the values for the elastic moduli

are more stable and converge on a global minimum if the least squares difference value is able to converge to a very small number.

As can be seen from the results, the solution depends strongly on the chosen convergence criterion. High values for the convergence criterion (>10) stop the calculation too early, resulting in too few iterations being carried out and an over-estimation of the seismic velocity. As the final value that the least-squares was required to reach reduces in absolute value, the result for the estimated seismic velocities converges to a stable final result. Based on these tests the final convergence criterion for the least-squares calculation, at which convergence is said to have been attained, was set to be 0.01Pa.

The following images show the results from the elastic modulus and seismic velocity estimation method developed for this thesis. The first two images, figures 4.6 and 4.7, are the results of a conversion from 1D temperature and melt fraction profiles calculated by the thermo-mechanical model into 1D velocity profiles through the centre of the modelled pluton.

Figure 4.6 is for a purely thermal numerical simulation carried out by the thermo-mechanical model using the low-frequency approximation to the solution for elastic moduli. Melt segregation terms in the governing equations were switched off so as to produce results that were directly comparable with previous models, specifically that of Paulatto et al. (2012) figure 12a. The simulation was run for a total of 23 ka and used two separate episodes of repetitive sill emplacements.

The first set of emplacements began at $t = 0$ and ran for 4 ka emplacing 300 m thick sills every 400 years to give a total 1D emplacement rate of 750 mmpa. 3 km of melt were emplaced in total via under accretion starting at 5.5 km depth in the first intrusion episode. A resting period of 15 ka then occurred during which the equations for heat diffusion were still solved and the resulting melt fractions from the purely thermal calculations were updated over time. At a run time of 19 ka a second emplacement episode began in the numerical simulation exactly identical to the first. Sills from the second set of emplacements via under accretion displaced deeper nodes by the thickness of an individual sill at each intrusion, thereby pushing down the remnants of the first emplacement episode in the process. This gave a final total intruded pluton thickness of 6 km. Intruded sills were set to have an initial melt fraction of 0.35.

Outputs from this purely thermal simulation in the thermo-mechanical model are produced at the end of the total 23 ka run time. At approximately 8.5 km depth evidence of the final sill emplacement can

be seen in the middle graph showing the final melt fractions. The two emplacement episodes give a distinct profile in the final temperature solution, which has two clearly defined perturbations to the standard geotherm.

Melt fraction values in figure 4.6 also have two clearly defined regions; 6 - 9 km depth where the most recent intrusions occurred and melt fraction is close to the original sill melt fraction (0.35), and 9 - 12 km depth where the melt fraction has decreased below 0.2 due to cooling. Due to the nature of the purely thermal model and the linear relationship between temperature and melt fraction, the depths of the perturbations in the melt fraction and temperature solutions directly correlate.

Seismic wave velocity results estimated from the 1D temperature and melt fraction profiles also show two distinct regions in the shallow crust. At 6 - 9 km below the surface the P-wave velocity decreases significantly due to the inverse relationship between increasing presence of melt and seismic velocity. A second, less pronounced low velocity zone exists between 9 - 12 km depth, relating to the first intrusion episode which has cooled and has a significantly lower melt fraction.

Bulk modulus values were calculated only in the emplacement zone and the region immediately surrounding the emplacement zone to increase the efficiency of the calculations. This can be seen from figure 4.6 to correspond to the region where a velocity anomaly was calculated. The bulk modulus increases with depth due to the increase in pressure. The final result can be seen to be highly dependent on the temperature and melt fraction results, with the region of high melt fraction (0.35) and high temperature between 6 - 9 km depth having a lower bulk modulus than the deeper region where melt fractions are much lower, <0.2 .

Results shown in figure 4.7 are at a run time of 23 ka for a numerical simulation identical to that in 4.6 where melt segregation and reactive flow have been accounted for by including those terms in the governing equations of the thermo-mechanical model. Despite the initial sills having a melt fraction of 0.35, as in figure 4.6, much higher average melt fractions can be seen in figure 4.7 when melt segregation is included in the calculations. All inputs for the models used to create figures 3.6 - 3.10 are given in table 4.2.

There are still two pronounced perturbations to the geotherm in the final temperature solution but the shallower solution, resulting from the most recent intrusion episode shows a much more complex and less smooth profile. This is also true of the melt fraction solution which shows seven distinct high melt fraction layers. The first three high melt fraction layers, between 5.5 - 6.5 km are separated only

by very thin low porosity layers. Below this, between 6.5 - 9 km depth we see three very distinct high melt fraction layers. The final sill emplacement, with a melt fraction of 0.35, at approximately 8.5 km depth is less pronounced in this profile due to the higher melt fractions in the system that mask its presence.

The most notable feature of the melt fraction results shown in figure 4.7 is the final, and deepest, high melt fraction layer that occurs between 9 - 10 km. The melt has accumulated over time and is at a much shallower depth than in figure 4.6. The melt fraction profile in 4.7 is also a lot less smooth due to the dynamic nature of melt segregation and the binary eutectic phase diagram used to calculate the evolution of melt fraction through time from the enthalpy and temperature results. The high melt fraction layer between 9 - 10 km depth varies in the value of melt fraction throughout the layer and this can be seen to correlate with the SiO_2 results shown in figure 4.8. In particular, the high silica content correlates with high melt fractions where temperatures are lower due to cooling after the first emplacement episode at 9 - 10 km depth. The initial silica content of the emplaced melt was set to be only 50% however the silica content of the country rock was set at 62.5%. As the melt migrates through the system it comes into contact with progressively cooler temperatures and evolves chemically with the silica remaining in the melt phase due to its low solidus temperature. Variation in the bulk modulus values throughout the emplacement zone correlates with the layers seen in the melt fraction results.

Results from the method for interpolation of the 1D velocity results from figure 4.6 into a 2D velocity profile can be seen in figure 4.9. The velocity results show a large low velocity zone in the shallow crust between 6 - 9 km and another, less pronounced low velocity zone between 9 - 12 km. These regions where the seismic wave speed has been calculated to be lower than the background velocity correlate with the emplacement zone. The velocity anomaly (figure 4.9 is 2 km wide, corresponding with the dimensions of the pluton produced by purely thermal modelling and shown in figure 12a of Paulatto et al. (2012). The extent of the velocity anomaly can be seen in figure 4.9 b). The largest value for the velocity anomaly is -1.32 km s^{-1} , at the point of the most recent sill intrusion at 9 km depth.

Interpolation between the 1D velocities and the background velocity gradient results in the smoothed edges of the intruded pluton that can be seen in figure 4.9. The diffusion distance from the edge of the pluton resulting from calculations made by the purely thermal model is less than 500 m across the entire height of the low velocity zone. The vertical extent of the velocity anomaly is much greater than the size of the emplacement zone, extending from approximately 3 km depth to 13.5 km.

Figure 4.10 shows the result of interpolating the 1D velocity results from figure 4.7 where melt segregation was taken into account. The most recently emplaced sill can be seen at approximately 9 km depth in the 2D velocity profile. The layers observed in figure 4.7 can clearly be seen in the 2D velocity profiles. The largest velocity anomaly, -2.49 km s^{-1} , is much larger when melt segregation is taken into account compared to that of the purely thermal model. Rising porosity waves can clearly be seen as individual low velocity anomaly regions in both figure 4.10 a) and b).

The background velocity gradient can be seen from both figure 4.9 and 4.10 to be high for the shallow crust, with a maximum value of 7.5 km s^{-1} reached at a depth of 21 km. This is due to the steep gradient used in the numerical simulation and the velocity conversion. The Moho for these examples was set to be shallow at 21 km depth, at the base of the plotted profiles, with the background velocity gradient set at 0.2 s^{-1} .

Figures 4.6 and 4.7 use the low-frequency approximation to the solution for the elastic moduli calculation. The low-frequency approximation assumes that melt pockets are connected via flow along the grain boundaries, resulting in pressure imbalances caused by the passing wave being dissipated. As a result, the main difference between the high- and low-frequency approximation results is that the final estimation of the P-wave velocity anomaly is marginally reduced when Gassmann's fluid substitution is used in the low-frequency approximation. The seismic velocities calculated in both the purely thermal low-frequency model (figure 4.9b) and the thermo-mechanical low-frequency model (figure 4.10b) have slightly lower bulk modulus values when calculated using the low-frequency approach described above in the method for the composite.

P-wave velocity in the purely thermal model is reduced by as much as -1.32 km s^{-1} , while in the thermo-mechanical model, an anomaly as large as -2.49 km s^{-1} can be seen in the lower half of the profile between 9 - 10 km. This corresponds to the region in figure 4.7 where the bulk modulus is reduced to 12.7 GPas. The overall trend of a broad low velocity zone in the purely thermal results compared to layers of high and low velocity anomalies in the thermo-mechanical results prevails across both the high- and low-frequency approximations.

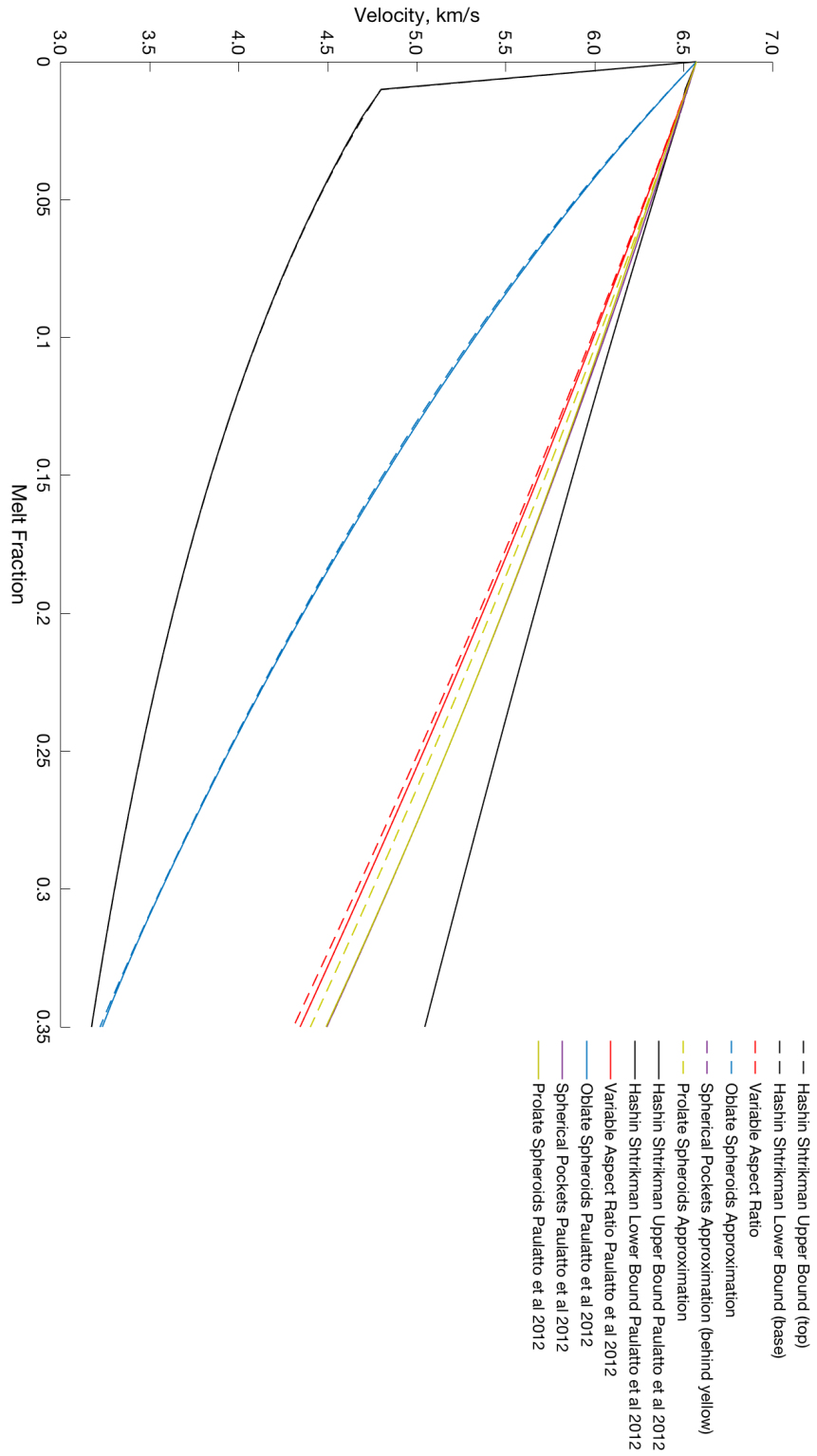


Figure 4.3: Test on the high-frequency approximation to the solution for seismic p-wave velocity from calculations of the elastic moduli based on melt fractions. The results from the velocity conversion developed for this thesis, dashed lines, are plotted against those of Paulatto et al. (2012) with the latter shown by solid lines. It can be seen that there is a very close match between the two approximations with the calculation of the Hashin-Shtrikman bounds matching exactly. The slight discrepancies can be explained by the use of different initial parameters in some of the cases plotted as the exact values used by Paulatto et al. (2012) were not known. The case for the spheroidal pockets approximation, purple, is hidden by the prolate spheroidal case of Paulatto et al. (2012).

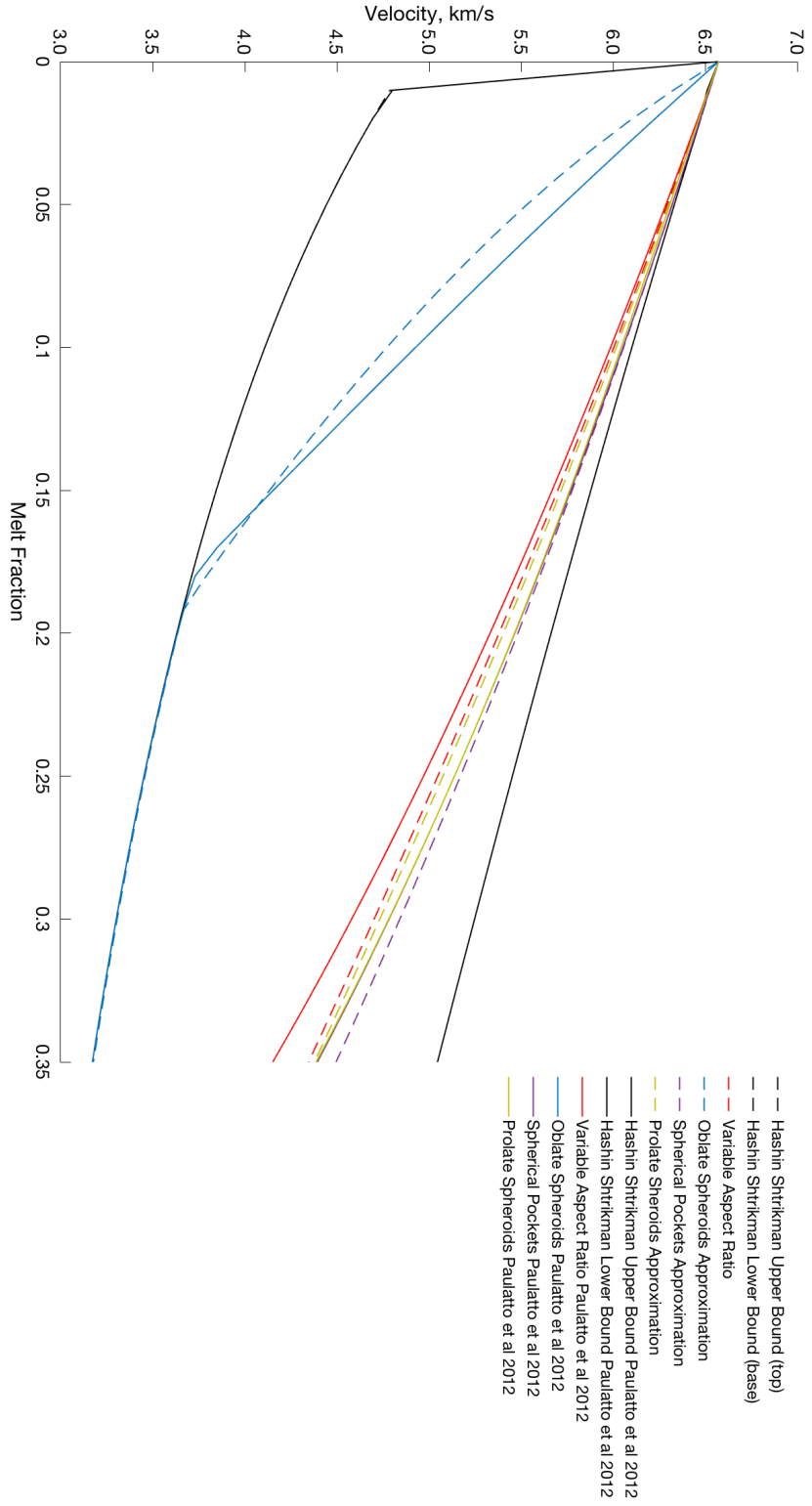


Figure 4.4: Test on the low-frequency approximation to the solution for seismic p-wave velocity from calculations of the elastic moduli based on melt fractions. The results from the velocity conversion developed for this thesis, dashed lines, are plotted against those of Paulatto et al. (2012) with the latter shown by solid lines. It can be seen that there is a very close match between the two approximations with the calculation of the Hashin-Shtrikman bounds matching exactly. The slight discrepancies can be explained by the use of different initial parameters in some of the cases plotted as the exact values used by Paulatto et al. (2012) were not known. In addition, for the case of the oblate spheroids approximation, it is possible that a different determination of the melt geometry may have been used.

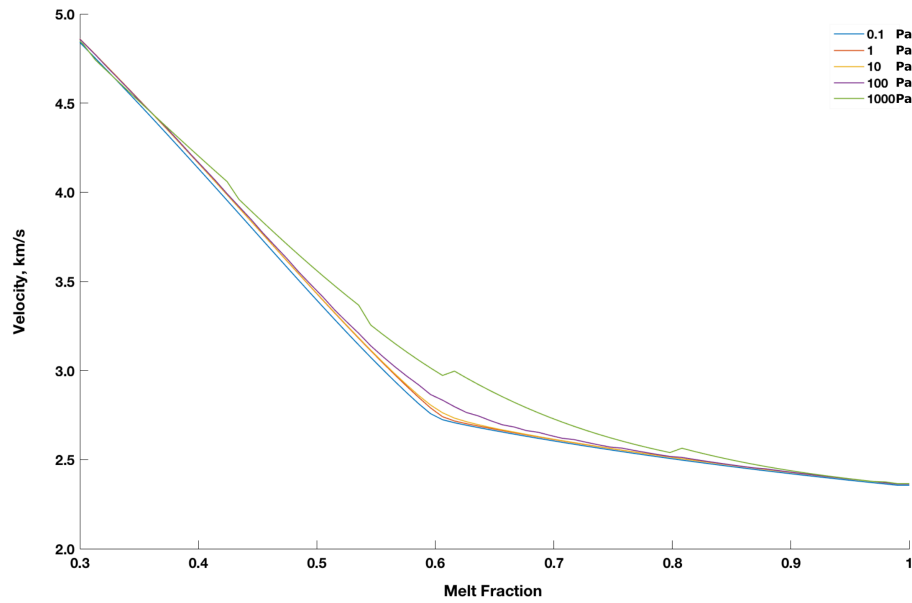


Figure 4.5: Least squares convergence test on velocity approximation. Calculated seismic velocities can be seen to be strongly dependent on the value at which convergence of the least-squares difference is determined to have been reached. The smaller the value of the least-squares convergence criterion, the lower the final estimated seismic velocities.

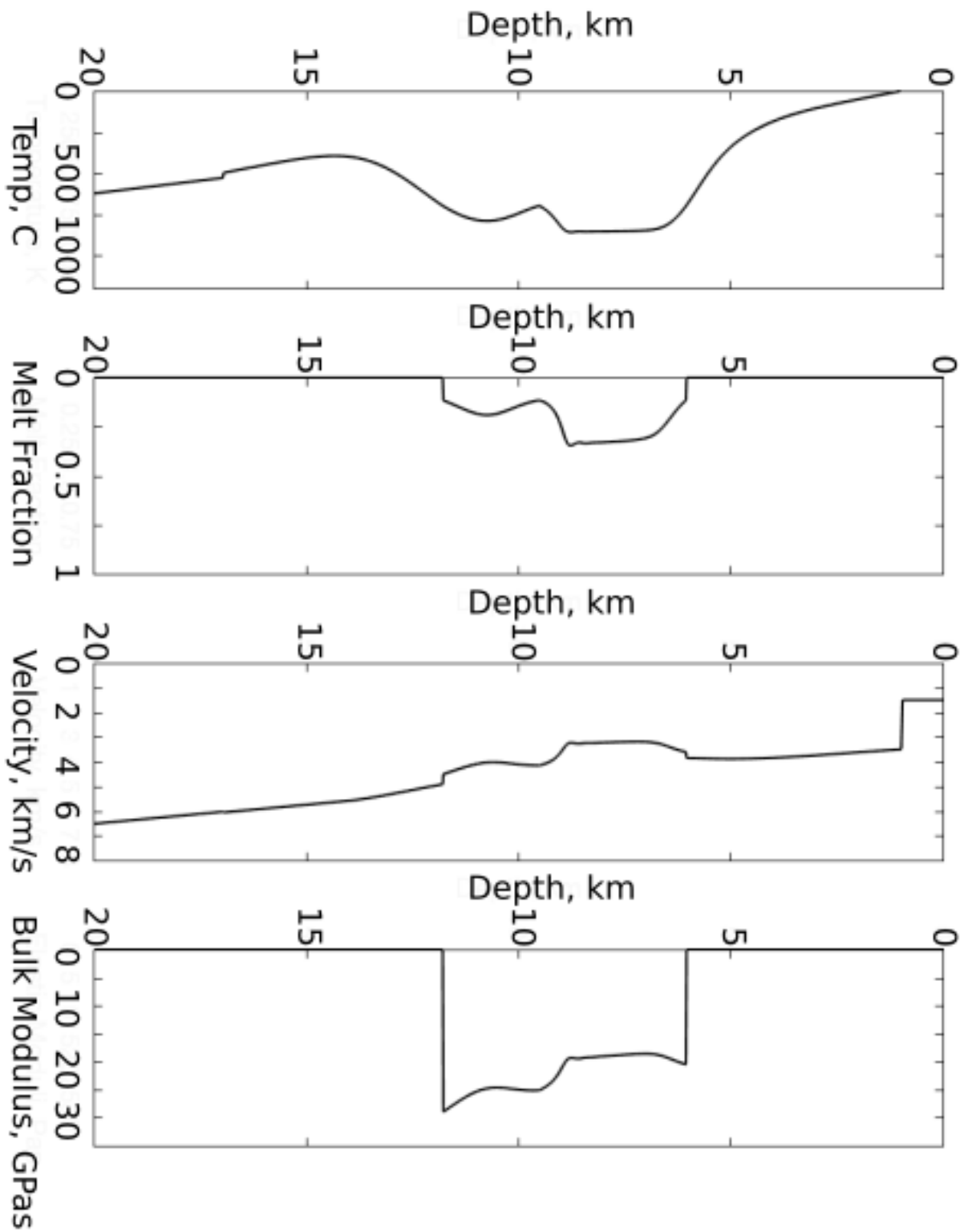


Figure 4.6: 1D profiles showing the P-wave velocities resulting from the calculation of the elastic moduli from the 1D temperature and melt fraction results of the thermo-mechanical model developed from purely thermal inputs, i.e. the melt segregation terms were switched off. The low-frequency approximation to the self-consistent approach of calculating elastic moduli was used. Two sets of emplacement routines occurred with an interval of 15 ka. Both emplacements were for 10 individual 300m thick sills at 750mmpa.

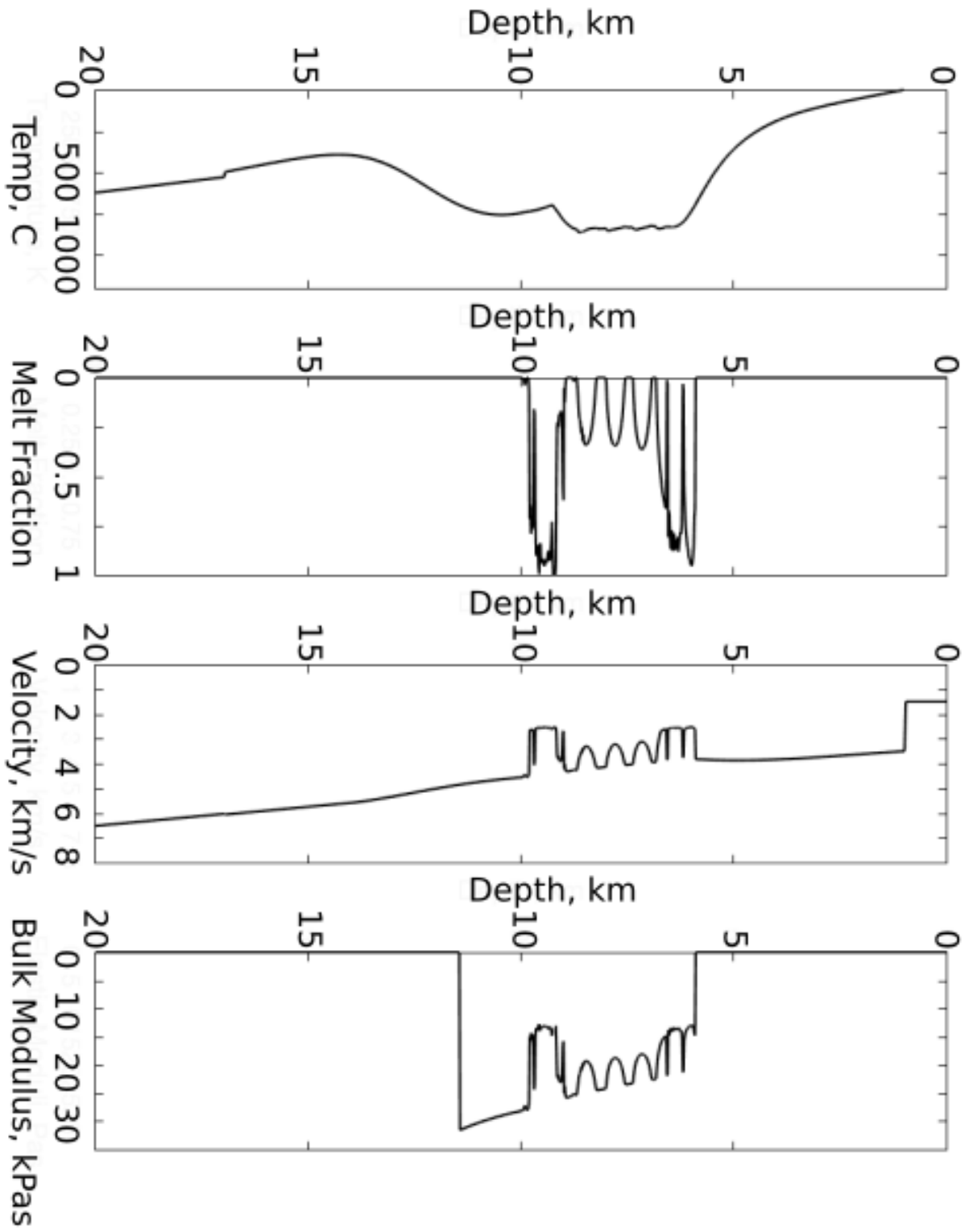


Figure 4.7: 1D profiles showing the P-wave velocities resulting from the calculation of the elastic moduli from the 1D temperature and melt fraction results of the thermo-mechanical model where melt segregation was taken into account during the numerical simulation. The low-frequency approximation to the self-consistent approach of calculating elastic moduli was used. Two sets of emplacement routines occurred with an interval of 15 ka. Both emplacements were for 10 individual 300m thick sills at 750mmpa.

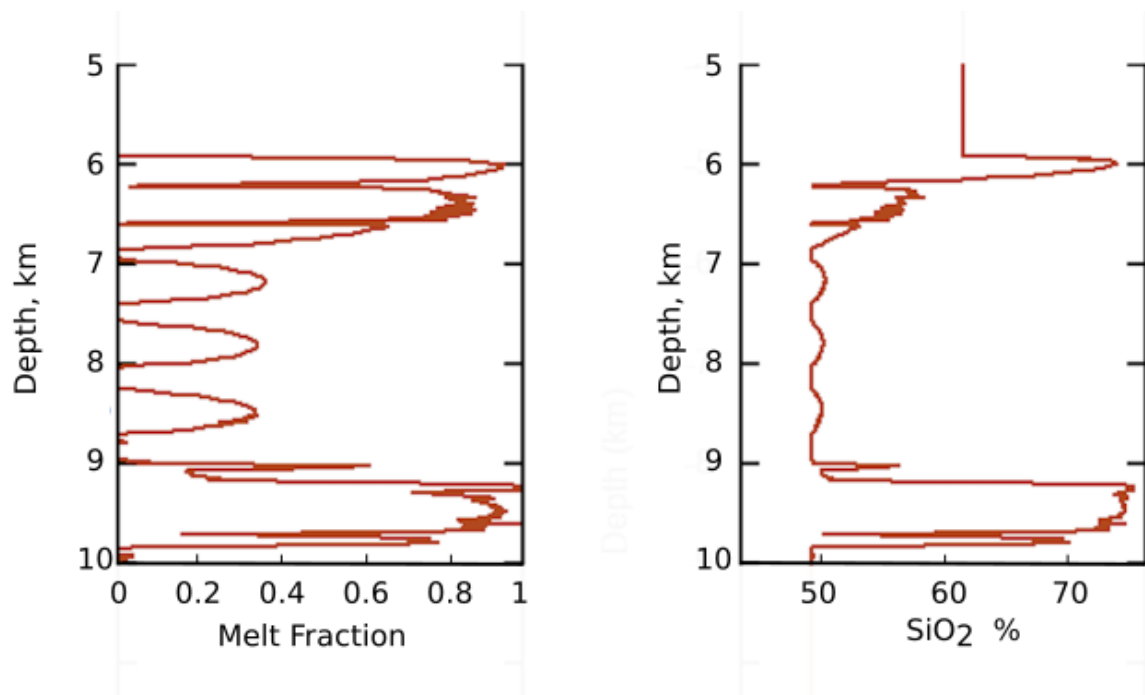


Figure 4.8: Melt fraction and silica content (%) of the system between 5 - 10 km depth at the final run time of 23 ka. The high melt fraction layers can be seen to correlate with the high silica content regions in the crust.

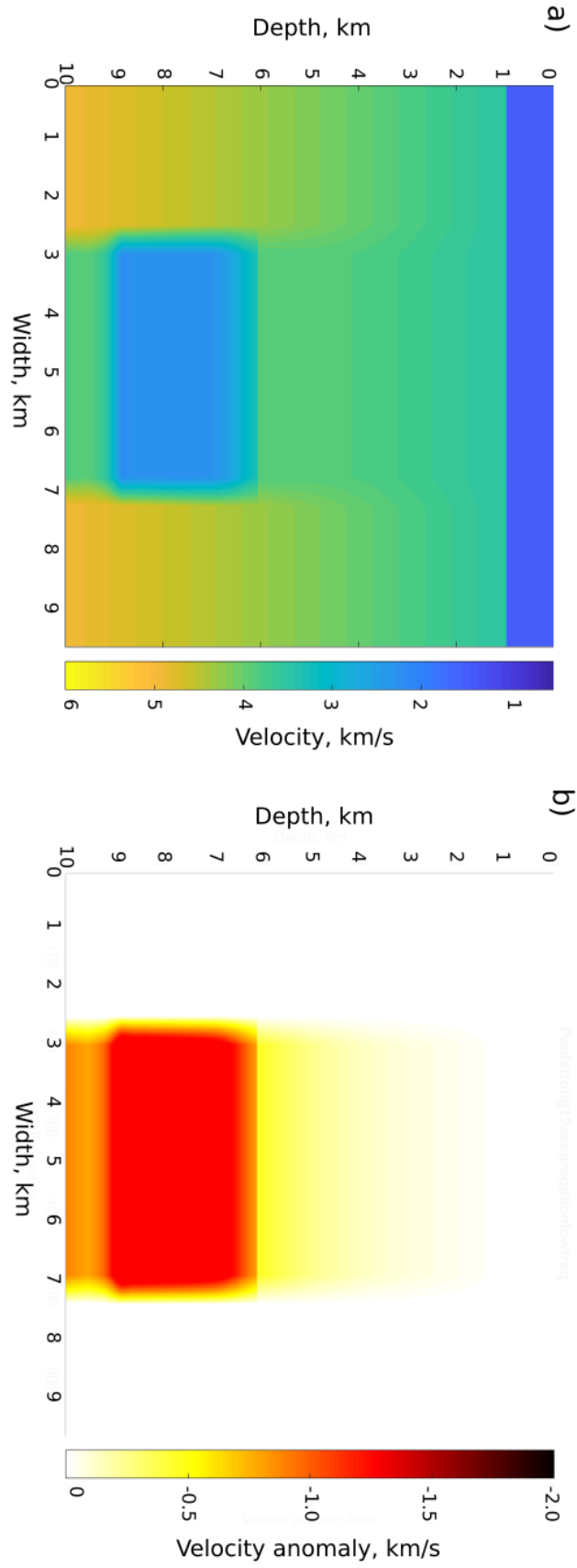


Figure 4.9: a) Velocity profile derived from the 1D results of the thermo-mechanical model when the melt segregation terms in the governing equations are switched off. The inputs used for the thermo-mechanical model in this example match those of Paulatto et al. (2012) figure 12, using the low-frequency approximation to the self-consistent approach of calculating elastic moduli. The final emplaced pluton is 2 km in radius. Two intrusion episodes of 300 metre thick sills emplaced every 400 years via under accretion for 4 ka occurred, with an interval of 15 km between the two episodes. Both intrusion episodes began at 5.5 km depth. b) Velocity anomaly for the purely thermal model at the low-frequency approximation. The large negative velocity anomaly corresponds to the region of high temperatures and melt fractions found by the thermo-mechanical model when the melt segregation terms in the governing equations are switched off.

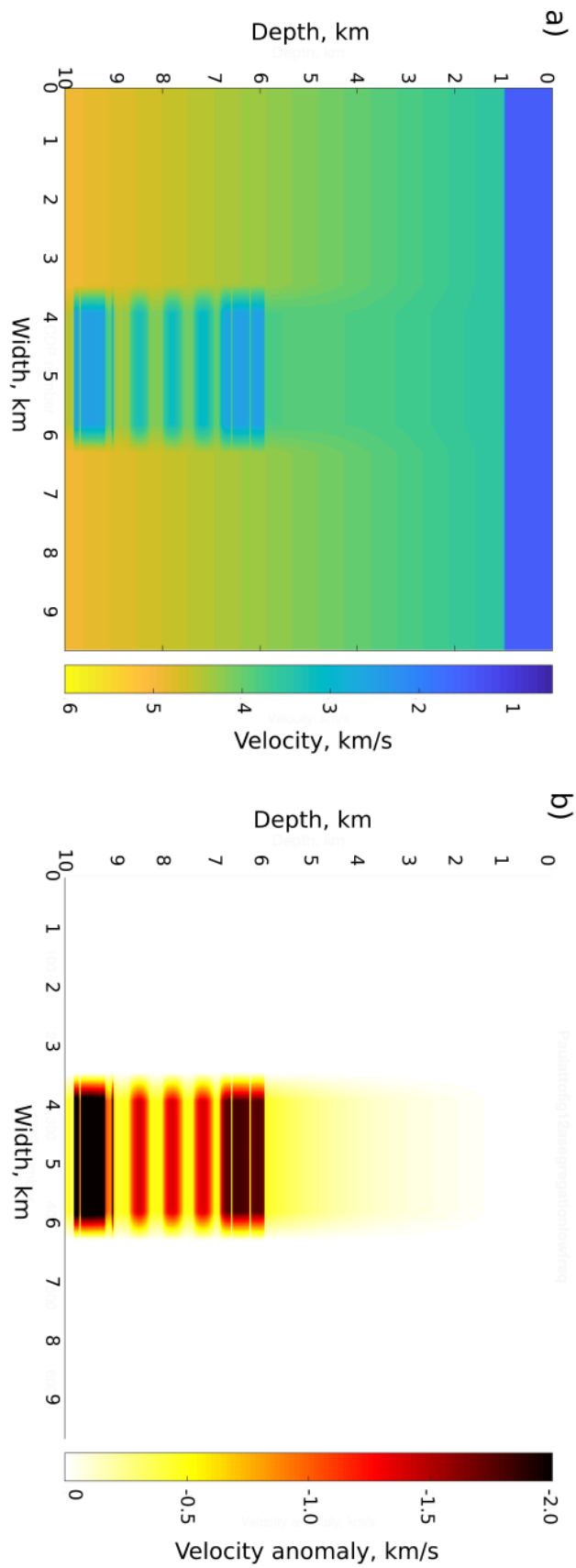


Figure 4.10: a) Velocity profile derived from the 1D results of the thermo-mechanical model when melt segregation is accounted for using the same inputs as for figure 4.9 using the low-frequency approximation to the self-consistent approach of calculating elastic moduli. The final emplaced pluton is 2 km in radius. Two intrusion episodes of 300 metre thick sills emplaced every 400 years via under accretion for 4 ka occurred, with an interval of 15 ka between the two episodes. Both intrusion episodes began at 5.5 km depth. b) Velocity anomaly for the thermo-mechanical model using the low-frequency approximation. The largest negative velocity anomalies are associated with the regions of highest melt fraction. The three lower negative velocity anomalies (approximately -1.5km/s) in the centre of the intruded pluton correspond to rising porosity waves of melt created by buoyancy-driven segregation in the incubated emplacement zone.

Unit	Value
Sill thickness (m)	300
Emplacement rate (mmpa)	750
Melt fraction	0.35
Initial emplacement depth (m)	5000
Time interval between emplacement (yrs)	400
Total run time of simulation (yrs)	23000
Time interval between episodes (yrs)	15000
Thermal conductivity ($\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$)	3.0
Latent heat of fusion ($\text{Jkg}^{-1}\text{K}^{-1}$)	550000
Pluton width (m)	1000
Total emplaced thickness (m)	6000
Liquidus temperature (K)	1223.15
Solidus temperature (K)	973.15
Density of solid (kgm^{-3})	2500
Density of melt (kgm^{-3})	2000
Density of sea water (kgm^{-3})	1000
Bulk modulus melt (GPa)	12.7
Shear modulus melt (GPa)	0

Table 4.2: Parameters used to produce figures 3.6 - 3.10 using inputs taken from Paulatto et al. (2012) in order to be able to make a fair comparison.

4.4 Discussion

Estimating seismic velocity values in the crust from temperature and melt fraction results requires a number of assumptions to be made for parameters including, but not limited to, the background velocity gradient, the background temperature gradient, the thermal conductivity of country and intruded rocks, and the density of the country and intruded rocks. When coupled with the uncertainties in the calculation of the elastic moduli it is clear that seismic velocity estimates are associated with quite large error bars. Differences in initial input values and adopted methods make it difficult to benchmark exactly against previous work however figures 4.3 and 4.4 show a good match to the elastic moduli calculations of Paulatto et al. (2012).

Due to the uncertainties involved, the 2D P-wave velocity profile calculated in figure 4.10 is considered to be a first order approximation to the true velocity anomaly. Further tests, carried out in chapter 4 of this thesis, are required to determine the extent to which the velocity estimates are capable of matching observed data.

The velocity anomaly found using segregation is a lot more complex than the broad low velocity zone seen in both purely thermal models. Layers of high melt fraction correspond to the largest absolute velocity anomalies in figure 4.10, where segregation was accounted for in the modelling process. The grid spacing for the velocity model is chosen to be 15 metres both horizontally and vertically as, later in the thesis (chapter 5), recovery of the fine-scale velocity structure will be attempted using full-waveform inversion. For crustal scale travel-time tomography grid spacings are generally much larger than this, on the order of 50 to 100 metres, in accordance with the resolution of the technique (Morgan et al., 2016).

There is also a clear difference in the final interpolation between purely thermal modelling and thermo-mechanical modelling results. In particular, the regions in the thermo-mechanical model where high melt fractions have accumulated via segregation result in a smaller diffusion distance and less smoothing at the edges of the intrusion zone. This is due to the lower residence time of the melt in the high melt fraction layer in comparison to the overall modelling time. A thin low velocity layer with sharp edges can clearly be identified at approximately 9 km depth in figure 4.10. This layer corresponds to the high melt fraction layer seen at 9 km in figures 4.8, and 4.6. As melt has accumulated over time in the region during continuous melt segregation, the time for which melt has been present in this layer is significantly less than the total time over which emplacements have occurred.

In addition, the high level of SiO_2 in this layer (75%) means that the melt at 9 km depth is more felsic, with a rhyolitic composition, and therefore has a lower melting temperature than both the surrounding country rock and the originally emplaced basalt. This melt-rich layer therefore exists for a longer duration during cooling as can be seen from the corresponding 1D temperature values at 9 km in figure 4.7. Calculated diffusion distances for the interpolation depend on the temperature difference as well as the residence time (equation 4.27), resulting in a smaller diffusion distance and less smoothing for the high melt fraction layer.

Comparison between figures 4.6 and 4.7 clearly shows the extent to which the bulk modulus values depend more strongly on the presence of melt rather than on changes in temperature for the high-frequency approximation. Sensitivity in the bulk modulus calculation directly translates into a stronger dependence on melt fraction for the final velocity values. The dependence of the velocity anomaly on melt fraction is even more pronounced in the low-frequency approximation. This relationship justifies the separate treatment of the anomalies caused by variations in temperature and melt fraction distribution. The difference in the melt fraction at 9 km between the purely thermal and the segregating cases is 0.65, whereas the difference in temperature is negligible. The influence of the presence of melt on final velocity values can therefore be seen to be very strong, with small changes in melt fraction values having a large effect on the P-wave velocity estimation.

Sensitivity of the elastic moduli and estimated seismic velocity values to the presence of melt is even more pronounced in the low-frequency approximation simply because the relaxed modulus is always lower than the unrelaxed modulus. Due to the dissipation of energy through interconnected melt pockets, the seismic velocity is greatly affected by the presence of melt in the low-frequency approximation. Modelling interconnected melt pockets results in negative velocity anomalies as large as -4.3 kms^{-1} in figure 4.10 in the accumulated high melt fraction layer between 9 - 10 km. This compares to a maximum velocity anomaly in this region of only -1.2 kms^{-1} for the purely thermal case in figure 4.9.

The low temperature values resulting from heat diffusion away from the region after the final high temperature, high melt fraction emplacement in the purely thermal model results in low melt fractions and a smaller negative velocity anomaly. In contrast, the same temperatures are able to sustain a large accumulation of melt in the thermo-mechanical model due to the use of the binary eutectic phase diagram for the melting relationship. As heat diffuses away from the region after the final sill emplacement of the first repetitive sill emplacement episode at 4 ka, the purely thermal model is no longer able to generate melt. However, the thermo-mechanical model continues to allow the

melt to segregate at low melt fractions and accounts for the compositional evolution of the melt as it maintains thermal and chemical equilibrium of the system, producing the observed high melt fraction lenses.

While the purely thermal modelling results in figure 4.6 show direct correlation between the regions of high temperature and those of high melt fraction due to the direct correlation in the linear melting relationship used, the segregation modelling results in figure 4.7 show decoupling between the location of highest melt fraction and the location of highest temperature. It is therefore difficult to separate the influence of temperature from that of melt fraction in the purely thermal cases whereas in figure 4.7 the different contributions to the final velocity anomaly from the two effects can clearly be seen.

4.5 Conclusion

The self-consistent approach of Berryman (1980a) was used in this thesis as it is valid for cases with high melt fractions such as those estimated in the thermo-mechanical model and it allows the simulation of realistic geometries by changing a single parameter: the aspect ratio of the spheroids. The fit of the benchmarking results against those of Paulatto et al. (2012) provides confidence in the approach used for the elastic moduli calculations. While discrepancies between the two results exist they most likely result from difference in initial input parameters in the models and the fact that Paulatto et al. (2012) were estimating the elastic moduli using a model derived from travel-time tomography coupled with a purely thermal model as opposed to from synthetic temperature and melt fraction data from a thermo-mechanical model.

While the interpolation from the 1D velocity estimations into a 2D profile is simply a first-order approach involving many simplifications, the results show that the method allows for clear distinction between the velocity anomaly caused by variations in melt fraction and those caused by variations in temperature. While Karato's equation to determine the effect of temperatures higher than the background temperature is an important step in the process, the overall anomaly due to temperature has been found to be much smaller than that due to the presence of melt. The method has been shown to be highly sensitive to the melt distribution due to the effect of the presence of melt on calculation of the elastic moduli and the effectiveness of the heterogeneous composite medium in transmitting seismic waves. As such, the results suffer from a degree of uncertainty because of the strong sensitivity of p-wave velocity to the melt geometry.

The governing equations have been shown to be sensitive to the geometry of the melt in the system. In particular, interconnected melt pockets have been shown to have a significant impact in reducing the estimated seismic velocities. Energy dissipation through interconnected melt pockets results in large negative velocity anomalies in regions of high melt fractions. During purely thermal modelling this produces large low velocity zones in the shallow crust. In contrast, thermo-mechanical modelling produces layered velocity anomalies corresponding with the high and low melt fraction layers. The following chapters build on the method outlined in this chapter to determine whether the seismic anomalies predicted by the thermo-mechanical model are distinguishable with seismic tomography.

Chapter 5

Modelling the Shallow Crust

5.1 Background

The spatial and temporal evolution of melt distribution in Deep Crustal Hot Zones (DCHZs) has been modelled extensively using both thermal and thermo-mechanical modelling (Annen and Sparks, 2002; Jackson et al., 2003, 2005; Annen et al., 2006; Solano, 2011; Solano et al., 2012, 2014). These studies of DCHZs have provided a wealth of information about magma ascent through the crust and the production of chemically evolved magmas from a single basaltic stock. While it is possible for mobile magmas to form within DCHZs and subsequently be capable of migrating upwards into the cooler, shallow crust without crystallising and stalling, the vast majority of pre-eruptive magmas have been found to have originated from storage regions in the shallow crust (Blundy and Cashman, 2001, 2008; Annen et al., 2015). The shallow zone, <8 km, in which eruptible magmas are stored in the crust is therefore of utmost significance when attempting to understand the spatio-temporal evolution of pre-eruptive melt distribution in the crust (Blundy and Cashman, 2008). For this reason, the following chapter focusses on modelling the shallow crust to enhance our understanding of the spatio-temporal evolution of melt distribution.

It is possible to obtain velocity models of the shallow crust using active source seismic data, which means we are able to make first-order comparisons between predicted seismic velocity models, like those presented in chapter 3, and tomographic velocity models from refraction data (Paulatto et al., 2012). Resolution is limited to half of the first Fresnel zone in travel-time tomography, where the Fresnel zone is defined as the volume around a ray, sampled by waves that all arrive in phase (within half a cycle) with the first arrival (Williamson, 1991; Williamson and Worthington, 1993; Rypina and Brown, 2007). As can be seen from equation 5.1, where t is the depth in time and v is the seismic velocity, the radius of the Fresnel zone, F_r , is inversely dependent on the seismic frequency, f , at which the waves travel through the Earth.

$$F_r = v \sqrt{\frac{t}{f}} \quad (5.1)$$

For deep experiments where the source-transmitter distance is large, velocities are higher, and the frequency of the wave is small, the Fresnel width becomes very large and the maximum possible resolution is compromised (Woodward et al., 2008). A refracted ray with a turning point at 12 km and a frequency of 10 Hz has an estimated Fresnel width of only approximately 5 km, making travel time tomography more suitable for imaging shallow velocity structure (Williamson, 1991). In

addition, there is relatively a much larger number of shallow seismic data-sets with which potential comparisons could be made between observed and modelled data. As such, shallow testing provides a better method for assessing the viability of the thermo-mechanical model in re-creating observed sub-volcanic structures.

This thesis concerns itself with the application of active refraction travel-time tomography to sub-volcanic exploration in the shallow crust. In essence, travel-time tomography is a model-building process where a forward problem is solved for synthetic travel times of seismic rays through a proposed model of seismic velocities. The inverse problem then involves comparing synthetic travel times with observed travel times from a seismic survey of the target region in the crust. Seismic energy from the source travels through the Earth and can be modelled as discrete rays. The travel time contains information about the nature of the media through which the ray travelled. By attempting to iteratively decrease the mis-match between the observed and synthetic travel times, a mathematical representation that is close to the true structure of the sub-surface can be reached (Rawlinson and Sambridge, 2003).

Final velocity models that are obtained from reduction of the misfit function in travel time tomography can be used to make interpretations about the composition of the imaging target (Zelt et al., 2003). Information about the thickness of sub-surface strata and their structural geometry can be determined from the velocity inversions produced, as well as estimates of various physical properties (Zelt, 1999; Rawlinson and Sambridge, 2003; Zelt et al., 2003). However, the final velocity and structural models produced using travel time tomography can be adversely affected by inadequate sampling of the target region (White and Boland, 1992; Zelt, 1999; Korenaga et al., 2000, 2002; Zelt et al., 2003). In addition, there is an inherent non-uniqueness of solutions, with a wide range of possible models being capable of satisfying the observed data (Zelt, 1999). Accuracy of the final results from travel time tomographic imaging therefore relies heavily on assumptions made in producing the original synthetic data for the forward problem as well as on the density of ray coverage (Tarantola, 1987; Zelt et al., 2003).

Application of travel-time tomography to sub-volcanic imaging has been a fairly recent development that has followed primarily from improvements in model resolution and improvements in coverage through the use of more closely spaced sources and receivers as well as by 3D surveys (Hole et al., 2005; Woodward et al., 2008). The design of seismic array geometries which are able to image beneath the complex overburden produced by igneous rocks in volcanic environments has made seismic tomography a viable method for sub-volcanic imaging (Ward et al., 2014). The highly crystalline nature of igneous rocks coupled with the sharp vertical lithological boundaries associated with volcanic plumbing systems

have made even shallow active volcanic sites difficult to image in the past. Crystalline structures and heterogeneous lithologies cause scattering of seismic energy as it travels through the media (Ziolkowski et al., 2003). The complex structural geologies in active volcanic regions and the associated steep velocity contrasts are problematic for conventional reflection seismic surveys but less so for refraction surveys (Mackenzie et al., 2005). However, rays from wide-angle surveys penetrate deeper into the crust and are able to sample beneath highly crystalline or partially molten overburdens at volcanic centres (Fliedner and White, 2001; Bouska, 2008; Morgan et al., 2013). As a result, wide-angled seismic data is capable of returning information to the surface about the internal structure of volcanic plumbing systems at a resolution of $10^2 - 10^3$ metres (Lizarralde et al., 2002; Mackenzie et al., 2005).

High-resolution travel-time tomography images of regions containing significant quantities of molten material in the shallow crust, which would potentially provide direct comparisons with synthetic results from the thermo-mechanical model, are rare (Alfaro et al., 2007; Lees, 2007; Paulatto et al., 2012). While a few seismic surveys have been conducted in island-arc settings, the majority have concentrated on large-scale crustal structure at relatively low resolutions (Shillington et al., 2004; Kodaira et al., 2007b,a; Takahashi et al., 2007; Calvert et al., 2008; Christeson et al., 2008). However, there have been a number of recent seismic surveys which were focussed on active volcanic centres in an attempt to quantify magma storage (Paulatto et al., 2012; Annen et al., 2014). In particular, a variety of work has been carried out at the Soufrière Hills Volcano, Montserrat, where recent activity, ongoing since 1995, has resulted in intensified interest in the region (Young et al., 1998; Mattioli et al., 2010; Kenedi et al., 2010; Paulatto et al., 2010, 2012; Annen et al., 2014).

5.2 Background of the study area

The Soufrière Hills Volcano is located on the southern end of the island of Montserrat in the Lesser Antilles ($16^{\circ}45'N$, $62^{\circ}12'W$). The island is approximately 16 km in length from N-S and only 10 km wide E-W, making it an easily viable target for wide-angled seismic surveys with offshore shots and onshore-offshore receivers. Its dimensions make it possible for marine seismic vessels to circumnavigate the island and for surveys to be carried out with relative ease.

There are three main volcanic centres on Montserrat and the island is comprised almost exclusively of volcanic deposits (Le Friant et al., 2004; Paulatto et al., 2010). The most southerly volcanic centre, Soufrière Hills Volcano, is the youngest (dating to at least 250 ka) and is currently still active while the more northerly Centre Hills and Silver Hills volcanoes have been extinct for the last 0.55 Ma

and 1.2 Ma respectively (Rea, 1974; Loughlin et al., 2010). Various studies have been conducted on the Soufrière Hills Volcano since the latest volcanic eruption started in 1995, including geological, geochemical, and geophysical observations in an attempt to better quantify the magma fluxes and understand its internal magmatic system (Le Friant et al., 2004; Kiddle et al., 2010; Paulatto et al., 2010; Shalev et al., 2010; Annen et al., 2014).

Evidence suggests that prior to the 1995 eruption, the Soufrière Hills Volcano had been dormant for over 300 years, with the last eruption resulting in the collapse of an andesitic dome (Young et al., 1998; Kiddle, 2011; Annen et al., 2014). Cycles of volcanic activity have been inferred to last between $10^3 - 10^4$ years, interspersed with much longer periods of inactivity (Le Friant et al., 2008). The last period of intense volcanic activity occurred between 31 - 17 ka ago, with the most recent period of volcanic activity having started approximately 6 ka ago with the collapse of the 1 km wide English's Crater on the east flank of the volcano (Roobol and Smith, 1998; Harford et al., 2002; Trofimovs et al., 2013). Four periods of increased seismic activity preceded the events of 1995, starting as early as 1897, with the most immediate seismicity prior to the onset of the 1995 eruption recorded between 1992-1994 (Shepherd et al., 1971; Aspinall et al., 1998). Activity in 1995 began with increased seismicity followed by phreatic eruptions, pyroclastic flows, and large scale collapse of an andesitic lava dome (Aspinall et al., 1998).

Between 1995 and 2008, activity was ongoing with three main episodes of lava-dome growth recorded using a combination of ground-based LiDAR data, photographic measurements, and seismic data from the Montserrat Volcano Observatory (Loughlin et al., 2010). Over-pressurisation of a magma chamber beneath the active centre at Soufrière Hills Volcano, caused by intrusion of molten material and degassing, has been invoked to explain the cycles of seismicity, uplift, and eruptions (Loughlin et al., 2010; Paulatto et al., 2010).

Geochemical and geological observations of amphiboles in the erupted material at the Soufrière Hills Volcano suggest that magma storage occurs primarily at depths of between 6 - 8 km (Barclay et al., 1998). This has been supported by deformation modelling carried out by Mattioli et al. (1998) using a point-source located at a depth of 6 km (Mogi, 1958). The broad-scale geology and structure had been modelled using gravity measurements and a large-scale 2D seismic refraction survey by Boynton et al. (1979) prior to the start of the latest eruption episode in 1995. Constraints for early modelling at Soufrière Hills Volcano came from a monitoring of volcano-tectonic swarms which resulted in a joint hypocentre-velocity structure inversion carried out by Villasenor et al. (1996). Further modelling by Hautmann et al. (2010b,a) has indicated that there may be a deeper magma storage reservoir located

at approximately 12 - 14 km depth. The presence of a deeper chamber has been supported by geodetic studies as well as by geochemical data that suggests shallow magma mixing.

Interpretation of various petrological data has inferred that there exist large variations in the temperatures at which distinct magmas have been stored over long periods of time, supporting the theory of a second, deeper magma reservoir (Murphy et al., 2000; Harford and Sparks, 2001; Couch et al., 2003; Humphreys et al., 2009; Annen et al., 2014). In addition, the petrology of erupted material is extremely heterogeneous, implying that there have been multiple episodes of cooling and reheating, most likely due to repetitive sill emplacements, which have resulted in complex mineral zoning and assimilation of the surrounding country rock (Devine et al., 1998; Murphy et al., 2000). It is important to note that stable isotope data collected by Zellmer et al. (2003a,b) has been used to conclude that crystal residence times in the shallow chamber at the Soufrière Hills Volcano are relatively short (<320 years). Erupted material which is of a broadly andesitic composition suggests that the parental magmas were generally of basaltic composition and have been mixed through convective stirring and magma movement through the complex volcanic plumbing system (Annen et al., 2014).

In December 2007, a small-scale, 3D active-source seismic survey termed the SEA-CALIPSO project was conducted in 3D to investigate the nature of the sub-volcanic system at the Soufrière Hills Volcano (Foroozan et al., 2010; Shalev et al., 2010). The aim of the experiment was to gain insight into the migration and distribution of melt between the mantle and the crust, and to investigate the geometry of the underlying geology at the active cone (Shalev et al., 2010). It followed the original Caribbean Andesite Lava Island Precision Seismogedetic Observatory (CALIPSO) project, set up in 2002, which was a collaborative effort across seven institutions, including the Montserrat Volcano Observatory, which investigated the dynamics at the Soufrière Hills Volcano (Linde et al., 2010).

The CALIPSO experiment used an array of equipment across four separate 200 metre deep boreholes as well as a number of shallower sites and monitoring stations at the surface (Mattioli et al., 2004). Data from three-component seismometers, tiltmeters, broadband dilatometers, and continuous GPS stations were integrated with strain-meter observations from the bore-holes, and surface geodetic and gas measurements to study the ongoing activity on Montserrat (Linde et al., 2010; Shalev et al., 2010; Voight and Sparks, 2010). Strain measurements from the 200m deep bore-holes provided an unprecedented insight into the potential geometry of the volcanic system. However, the non-uniqueness of the model geometries used to explain the observed strain measurements, and inconsistencies with geochemical evidence for the depth at which melt storage occurred, led to the conclusion that a seismic

survey was required to help distinguish between competing models (Linde et al., 2010; Annen et al., 2014).

The SEA-CALIPSO seismic survey was subsequently carried out to complement data from the original CALIPSO experiment and to give a better understanding of the nature of magma storage and variable seismic velocity zones in the crust below the Soufrière Hills Volcano. Given the limited resources available, the experimental array of seismometers was made to be as dense as possible and included both onshore and offshore active-source seismic stations. A marine seismic vessel was used with an eight-component GI airgun which shot at average intervals of 1 minute over the course of 77hrs to fire 4414 shots in total (Paulatto et al., 2010; Shalev et al., 2010). The array was towed at a depth of 10m below the sea surface at a speed of 2.3 ms^{-1} , to give a mean shot spacing from the offshore experiment of 139m (Paulatto et al., 2010). Ten ocean-bottom seismometers were deployed and the survey covered a total area of 50 x 40 km (Shalev et al., 2010).

The onshore component of the SEA-CALIPSO experiment included the deployment of two different seismic arrays; 28 three-component, short-period, 2 Hz seismograms were deployed over a regularly spaced grid in addition to 209 one-component, 4.5 Hz, geophone seismograms which were deployed along five separate transects that crossed the island (Paulatto et al., 2010; Shalev et al., 2010). Pre-existing seismic stations from the Montserrat Volcano Observatory also recorded shots fired during the SEA-CALIPSO project. The final geometry of the station arrays, ship track, and shot positions can be seen in figure 5.1 which has been adapted from Paulatto et al. (2010) and Shalev et al. (2010). Due to the ongoing activity at the Soufrière Hills Volcano it was not possible for seismometers to be deployed within the hazardous exclusion zone to the south of the island, so land-based seismometers are concentrated on the northern end of the island and the path taken by the marine vessel was focussed around the south-east of the island, as can be seen in figure 5.1 (Shalev et al., 2010).

Results from the SEA-CALIPSO seismic survey, figure 5.2, have been used for various travel-time inversions which span multiple different transects across the island (Paulatto et al., 2010, 2012; Annen et al., 2014). Consequently, there exists a variety of different 2D p-wave velocity models from the SEA-CALIPSO experiment which can be compared with the synthetic p-wave velocity profiles created by the thermo-mechanical model. The majority of the first-arrival travel time data observed was of relatively high quality and easily identifiable from the recorded seismograms (Paulatto et al., 2010, 2012). Ambient noise levels from ocean waves was found to be quite high, and stations in the north were affected less by attenuation of the signals as the volcanic deposits there are much older (Kenedi et al., 2010).

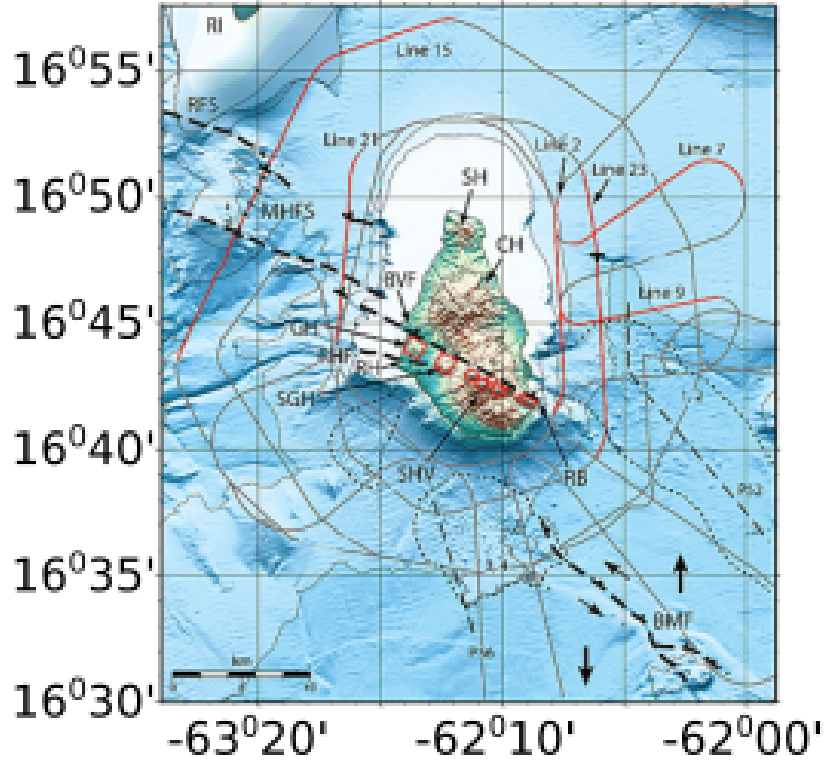


Figure 5.1: Adapted from Kenedi et al. (2010). Locations of the ocean bottom seismometers are shown as purple circles. The white triangles show the positions of the one-component seismometers, black triangles show the positions of the three-component seismometers. The ship tracks are shown surrounding the island and the major fault lines are depicted as thick dashed black lines running through the island. Volcanic centres are denoted on the southern half of the island with red circles and the Soufrière Hills Volcano is marked with an arrow labelled SHV.

Ray coverage for the inversion by Paulatto et al. (2012) is shown in figure 5.3 at both 2 and 7 km depth. This gives a good first estimate for the resolution of the model, with the densest coverage of rays found to be in the area immediately beneath the island at approximately 3 km depth (Paulatto et al., 2012). Resolution was determined to be highest between 2 - 6 km and deteriorated sharply below 7.5 km. Paulatto et al. (2012) used the regularised least squares approach of Hobro et al. (2003) to generate a seismic p-wave velocity model from travel time data recorded by the SEA-CALIPSO

seismic survey. The inversion process used an initial velocity model estimate based on work from previous studies, and then iteratively updated the starting model to reduce the misfit between the observed and modelled data.

In the velocity model obtained by Paulatto et al. (2012) there is a low-velocity anomaly beneath the Soufrière Hills Volcano between 6 and 8 km depth (figure 5.2) suggesting the presence of melt at these depths. Paulatto et al. (2012) found a large low velocity zone with a volume of approximately 100 km³ beneath the active volcanic centre at the Soufrière Hills Volcano. P-wave velocities were found to have been reduced by more than 0.5 kms⁻¹ across 20 km³ of the low velocity zone, corresponding to melt fractions of between approximately 6 - 10% in the region (figure 5.4). The low velocity zone is thought to correspond to the main region of magma mixing and storage at the Soufrière Hills Volcano and is approximately 4 km in diameter. It has been hypothesised that a second low-velocity zone, corresponding to a deeper reservoir, lies below this at approximately 12 km.

The p-wave velocity model was firstly used to estimate temperature across the volcano using the process outlined by Karato (1993). A self-consistent approach for determining the effective elastic moduli of multi-phase composites was then used which followed the method described by Berryman (1980a). The estimates for the bulk and shear moduli were then used to determine the corresponding range of possible melt fraction distributions beneath the Soufrière Hills Volcano. For a full description of the method see Paulatto et al. (2012). In effect, the process is exactly the opposite of that used in chapter 3 of this thesis which takes the results for temperature and melt fraction distribution from the thermo-mechanical model and solves for the elastic moduli and p-wave velocities. Final results for temperature and melt fraction estimates for the sub-volcanic region at Soufrière Hills calculated from the velocity model by Paulatto et al. (2012) are shown in figure 5.4.

Results from the analyses of the seismic velocities were then compared to numerical models of the evolution of melt distribution at the Soufrière Hills Volcano to investigate magma storage in the sub-volcanic crust (Paulatto et al., 2012). The numerical model of heat transfer and melt accumulation in the shallow crust at Montserrat developed by Paulatto et al. (2012) solves the heat diffusion equation using a finite difference scheme as described in equation 5.2, following the work of Annen (2009) (Annen, 2011; Paulatto et al., 2012; Annen et al., 2014). ρ is the density, C_p is the specific heat capacity, T is the temperature in Kelvin, t is time in seconds, ϕ is the melt fraction (dimensionless), L_f is the latent heat of fusion (or enthalpy of crystallisation), and κ is the thermal conductivity.

$$\rho C_p \frac{\partial T}{\partial t} + \rho L_f \frac{\partial \phi}{\partial t} = \kappa \Delta^2 T \quad (5.2)$$

Paulatto et al. (2012) discovered that high one-dimensional sill accretion rates, $>10^2$ mmpa, were required using repetitive sill intrusions in their thermal model to produce the volumes of crystal-poor magma needed to create a mobile magma capable of erupting (Annen, 2009). They determined that high intrusion rates of 750 mmpa were required in order to produce a velocity anomaly signature comparable to the one obtained by the inversion of the SEA-CALIPSO data shown in figure 5.2.

The high emplacement rates required in the model of Paulatto et al. (2012) were needed because the low temperatures within the shallow crust inhibit incubation of the pluton. Repetitive emplacements are eventually able to incubate the shallow crust over a long period of time when the background temperatures are increased within the shallow crust and can therefore sustain the generation of large volumes of melt (Annen, 2009, 2011).

Petrological data has determined that it is theoretically possible for melt to have been emplaced at the high one-dimensional rate of 750 mmpa used by Paulatto et al. (2012) to reproduce the low velocity signature seen in the travel time tomography inversion at the Soufrière Hills Volcano shown in figure 5.2a. Evidence for high rates greater than 10^2 mmpa has been found using geochemical and petrological data in certain cases before the onset of large, caldera-forming eruptions (Wilson et al., 2005). In the specific case of a caldera forming eruption, the volume of mobile eruptible magma is usually $>10^2$ km³ and is often crystal-poor and highly evolved in nature (Jellinek and DePaolo, 2003; Cashman and Giordano, 2014).

However, geochronologic data suggests that average 1D pluton emplacement rates over geological timescales are much lower than 10^2 mmpa and on the order of <10 mmpa (Annen, 2009). Plutons which have been uplifted and eroded down at the surface of the Earth, thereby making it possible to study them, have been determined by geochronology to result from emplacement episodes lasting many millions of years at low emplacement rates, much less than 750 mmpa (Coleman et al., 2004; Schoene et al., 2012). Various studies have determined that the shallow crust would not be capable of accommodating sustained high intrusion rates $>10^2$ mmpa over geological time scales due to the lack of space available in the crust (Weinberg, 1996; Vigneresse and Clemens, 2000). The large volumes of intruded melt at such high rates would produce a substantial, but as yet not observed, level of uplift per annum that would be measurable using synthetic aperture radar interferometry (Petford, 1996; Klügel et al., 2005). Furthermore, models of lithospheric flexure have shown that a key limiting

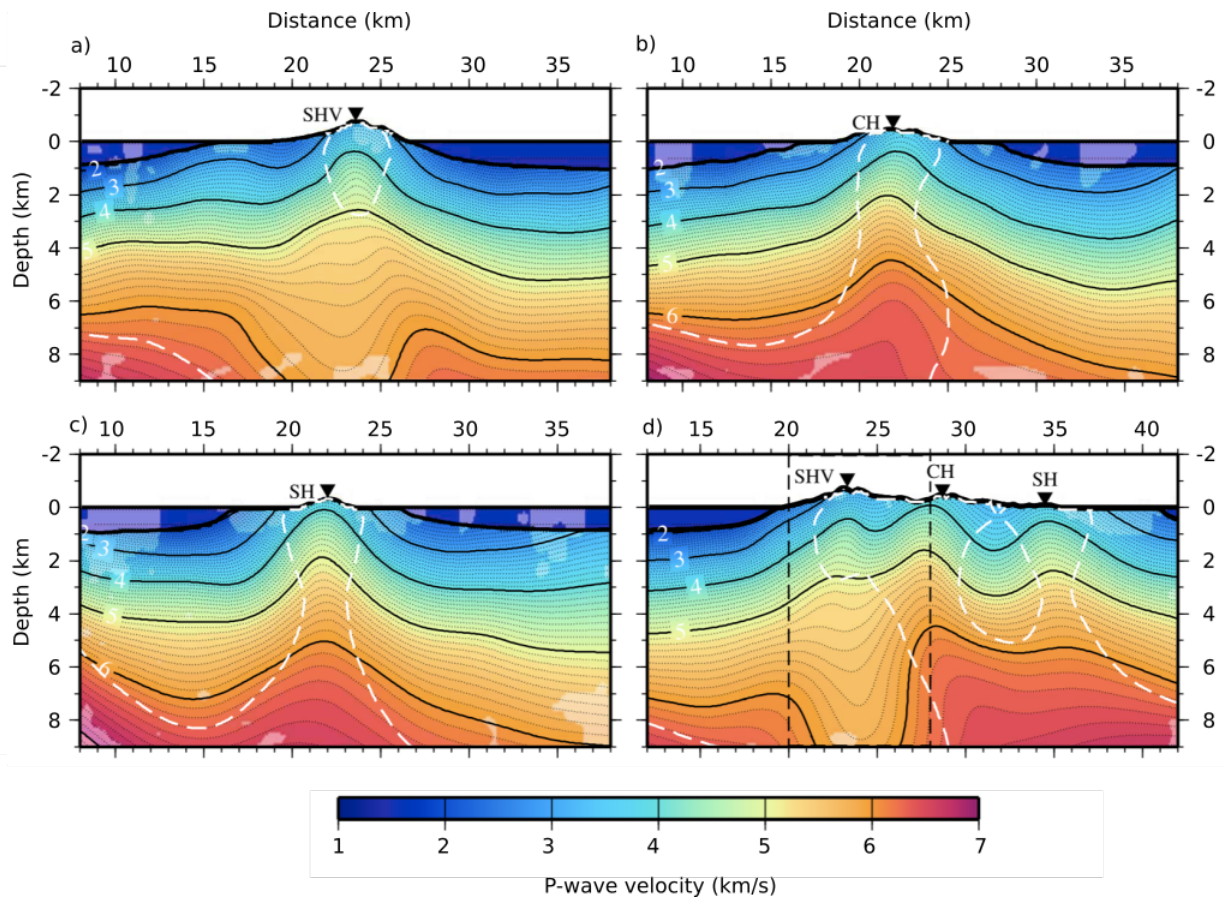


Figure 5.2: 2D travel time tomography inversions for p-wave velocity along two transects through the Soufrière Hills Volcano in Montserrat, taken from Paulatto et al. (2012). The 2D profiles relate to transects shown in figure 5.3. a) shows the results from the east-west transect along line A-A' through the Soufrière Hills Volcano, b) shows the results from the east-west transect along line B-B', c) shows the results from the east-west transect at the northern tip of the island along line C-C', d) shows the results from the north-south transect along line D-D'. The white dashed lines mark out high seismic velocity zones found at the core of each volcanic centre by Paulatto et al. (2012).

factor on the rate at which melt is able to be emplaced in the shallow crust is its cold and brittle nature (Vigneresse and Clemens, 2000; Galgana et al., 2011). Thus, it appears that models of melt distribution and accumulation in the shallow crust developed by Paulatto et al. (2012) and Annen et al. (2014) are incompatible with the low rates of crustal melt emplacement found using geochronology for igneous intrusions (Jackson et al., 2003, 2005).

Evidence suggests that both small eruptions and caldera-forming eruptions can be better explained by the evacuation of magma from multiple crystal-poor lenses of melt rather than from a single large chamber (Cashman and Giordano, 2014). In addition, the existence of compositional spatial variability in studied eruption sequences suggests that the melt resides in a transient sub-volcanic mush as opposed to the large, long-lived body of magma used to produce estimates of melt fraction

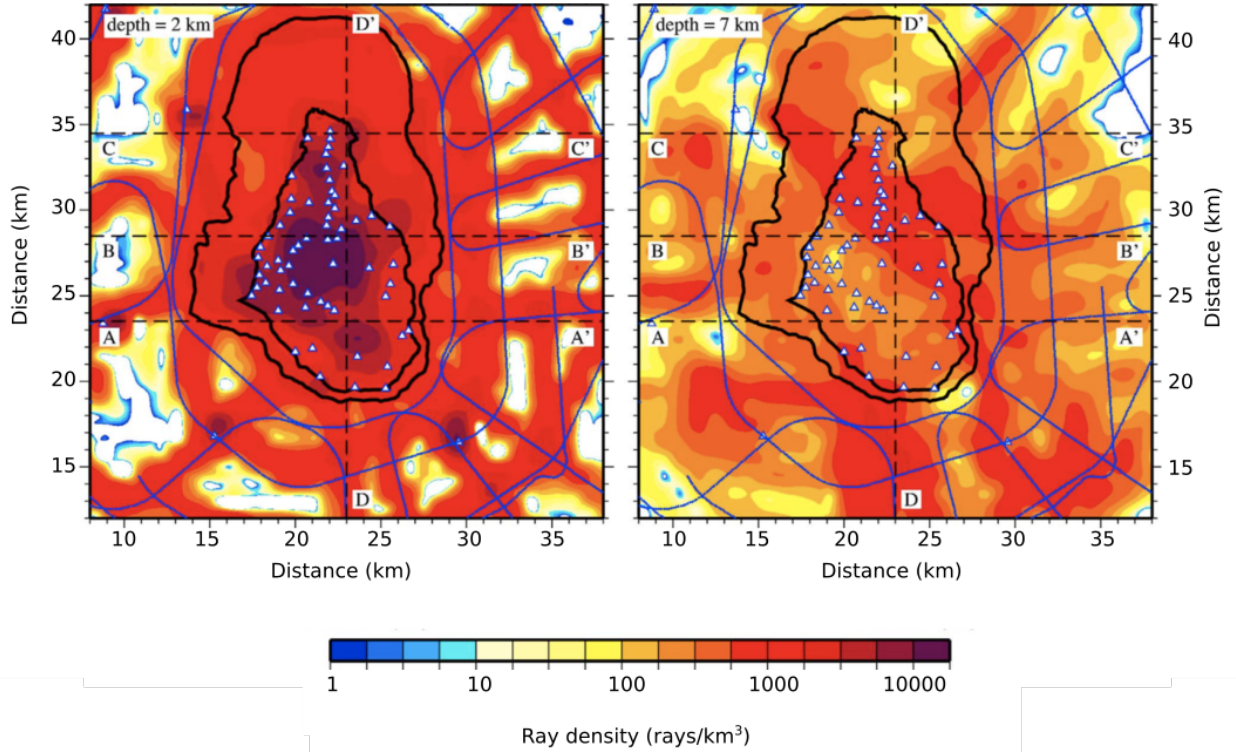


Figure 5.3: Horizontal sections showing ray density at 2km and 7km depths calculated by Paulatto et al. (2012). The transects from figure 5.2 are shown, with A-A', B-B', and C-C' running east-west and D-D' running north-south. Taken from Paulatto et al. (2012).

distribution to explain the velocity anomaly found at the Soufrière Hills Volcano by thermal models (Paulatto et al., 2012; Gualda and Ghiorso, 2013; Annen et al., 2014; Cashman and Giordano, 2014). Estimations for the long term average and maximum melt fluxes predicted by Annen et al. (2014) at the Soufrière Hills Volcano, using thermal modelling to reproduce the measured velocity anomaly, are significantly lower (average 1D flux of 30 mmpa) than those originally predicted by Paulatto et al. (2012). However, over intrusion time-scales greater than 100 ka, this thermal model is unable to match the temperature of the volcanic system inferred by petrological observations (Barclay et al., 1998; Devine et al., 1998; Murphy et al., 2000). As the thermal model cools it is unable to sustain melt production and so the entire modelled system solidifies (Annen et al., 2014). Therefore, it appears that attempting to reproduce the melt fraction and temperature distribution from a seismic velocity inversion at the Soufrière Hills Volcano using a purely thermal model would not capture the full nature of the dynamic system. In particular, the sill emplacement rates that are required in the thermal model shown in Paulatto et al. (2012) to produce the estimated melt signature calculated from the derived elastic moduli are likely to be substantially higher than the average rate at which melt intrudes into the shallow crust at the Soufrière Hills Volcano. Thermo-mechanical modelling,

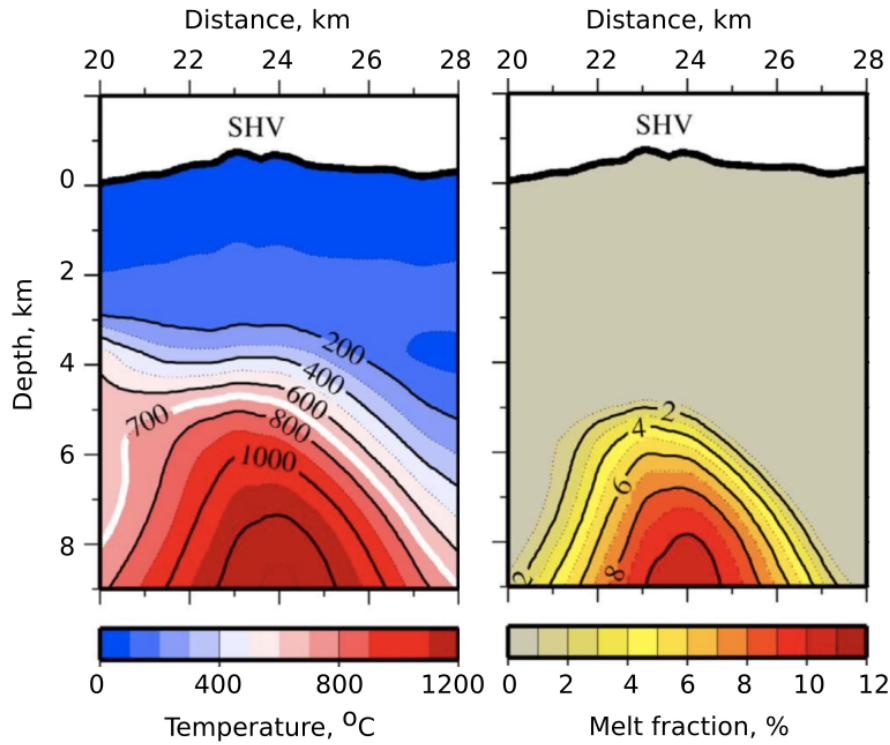


Figure 5.4: Final estimates for temperature and melt fraction beneath the Soufrière Hills Volcano calculated by Paulatto et al. (2012) from their p-wave velocity inversion of the SEA-CALIPSO seismic data. Melt pocket geometry was assumed to be spherical and interconnected. Adapted from Paulatto et al. (2012).

integrating melt segregation and reactive flow, has the potential to produce a result for melt content and geometry that is very similar to the purely thermal model using significantly lower emplacement rates.

To test this hypothesis it was necessary to first compare the thermo-mechanical model results of simulations in the shallow crust to those produced by Paulatto et al. (2012) using their purely thermal model. The method by which this was carried out and the results from the tests are described in the following sections of this chapter.

5.3 Method

5.3.1 Numerical modelling

Two significant adaptations were made to the thermo-mechanical model developed by Jackson et al. (2018) in order to model the shallow crust and benchmark the thermal solution against previous modelling. First, the input routine to the model, as shown in figure 2.3, was adjusted to allow for multiple emplacement episodes during the run time of the modelled scenarios. This was a simple adjustment that was made in order to match the input routines used by Paulatto et al. (2012) and Annen et al. (2014). Both studies utilise rest periods between separate episodes of repetitive sill emplacements in the shallow crust in order to try and match the recovered velocity model at the Soufrière Hills Volcano in Montserrat.

Secondly, the enthalpy solver in the thermo-mechanical model was changed to allow for sill emplacements to occur at melt fractions <1 . Previous versions of the thermo-mechanical model developed by Solano et al. (2012) and Jackson et al. (2018) only allowed for initial sill melt fractions of unity due to the method used to non-dimensionalise the system of general equations (Solano, 2011). However, the modelling conducted by Paulatto et al. (2012) used sill emplacements with initial melt fractions of 0.35 to reproduce the melt fraction distribution estimated by the conversion from the seismic velocity inversion of the SEA-CALIPSO data. As such it was necessary to re-design the non-dimensionalisation process to accommodate emplacements at melt fractions of less than one. This was done by scaling the non-dimensional enthalpy and temperature to the solidus values.

5.3.2 Seismic travel-time tomography

The first step was to reproduce the results of Paulatto et al. (2012) using the thermo-mechanical model with the same initial inputs. Table 5.1 shows the inputs used. These are taken from Paulatto et al. (2012). The next step was to convert the models of temperature and melt fraction obtained from the numerical simulations into seismic velocity using the approach described in Chapter 3. It was necessary to filter the final outputs of the derived velocity models to take into account the resolution of velocity models obtained from travel-time tomography. The numerical simulations used a very fine grid spacing to calculate the coupled system of equations for advection, diffusion, compaction, and segregation and produced a fine-scale velocity model with node spacing on the order of $10^{-1} - 10^0$ metres. In contrast,

the seismic velocity profile determined from the SEA-CALIPSO travel-time tomography inversion at Montserrat had a grid spacing on the order of $10^2 - 10^3$ metres. As a result, the high resolution velocity models produced from the thermo-mechanical modelling results were filtered using the `tomo2d` package developed by Korenaga et al. (2000).

The 2D p-wave velocity model developed using the method outlined in chapter 3 from the melt fraction and temperature distribution results from the thermo-mechanical model was first parameterised as a shear mesh in order to be used in the `tomo2d` inversion. Travel times and ray paths were then calculated by the `tomo2d` package which uses a combination of the ray-bending method and the shortest-path method (Korenaga et al., 2000). This hybrid approach makes `tomo2d` very efficient both in terms of the time taken for the calculations and the memory required (Korenaga et al., 2000, 2001).

The shortest-path, or graph, solution is initially used by `tomo2d` to develop a forward star representation of the ray paths (Korenaga et al., 2000). This essentially produces a map of the possible node connections along the grid and is able to provide a good first order estimate of the travel times between source and receiver pairs (Van Avendonk et al., 1998; Van Avendonk, 1998; Zhang and Toksöz, 1998; Korenaga et al., 2000). The order of the forward star approach is calculated by `tomo2d` based on the complexity of the initial velocity model supplied and the node spacing. A more complex model with a finer initial grid requires a higher order forward star, and therefore more computation time, to produce an initial estimate of the travel times (Korenaga et al., 2000). Due to the dominance of the vertical velocity gradient in the crust, the `tomo2d` software uses a forward star that searches in the vertical direction preferentially so as to reduce computation time (Korenaga et al., 2000). The initial estimate provided by the shortest-path method is then refined using the ray-bending method of Moser et al. (1992).

The ray-bending procedure converges on a final solution by iteratively minimising the travel times along ray paths using a conjugate gradient method (Moser, 1991; Moser et al., 1992). While it would have been possible to use a finite difference method to calculate the ray paths, the sharp velocity contrasts at the pluton edges would have caused significant inaccuracies in the travel time results (Vidale, 1988). Combining the shortest-path and ray-bending methods allows the `tomo2d` software to converge efficiently on a global minimum for the ray paths and final travel time estimates in the model without compromising on grid resolution (Korenaga et al., 2000).

A 2D velocity model was created from the background velocity profile for the calculations in chapter 3 and used as an initial reference velocity model for the inverse problem in `tomo2d`. A vector containing

Symbol	Unit	Value
z	Sill thickness (m)	300
r	Emplacement rate (mmpa)	750
ϕ_0	Melt fraction	0.35
x_0	Initial emplacement depth (m)	5000
dt_0	Time interval between emplacement (yrs)	400
t_{final}	Total run time of simulation (yrs)	23000
t_{int}	Time interval between episodes (yrs)	15000
k	Thermal conductivity ($\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$)	3.0
L_f	Latent heat of fusion ($\text{Jkg}^{-1}\text{K}^{-1}$)	550000
ω	Pluton width (m)	1000
z_{total}	Total emplaced thickness (m)	6000
T_L	Liquidus temperature (K)	1223.15
T_S	Solidus temperature (K)	973.15
ρ_s	Density of solid (kgm^{-3})	2500
ρ_m	Density of melt (kgm^{-3})	2000
ρ_w	Density of sea water (kgm^{-3})	1000
v_w	Seismic velocity in sea water (ms^{-1})	1500
K_m	Bulk modulus melt (GPa)	12.7
μ_m	Shear modulus melt (GPa)	0

Table 5.1: Parameters used in the thermal run of the thermo-mechanical model to benchmark against the results of Paulatto et al. (2012). The simulation used two emplacement episodes separated by a time interval, t_{int} . Sills were emplaced via under accretion.

the first arrivals is then mapped iteratively onto the Frechet derivative matrix by the tomo2d software until the model converges on a final velocity model (Korenaga et al., 2000). Inversions are often unstable when fine-scale grids are used, such as those employed in the calculations of the thermo-mechanical model, due to the restrictive singularity of the relationship on such small grid cells between the travel time residuals, the Frechet derivative matrix, and the perturbations in the velocity model (Toomey et al., 1994). Not only does an very fine mesh result in large calculation times but it is also often not possible for tomo2d to calculate the travel time residuals. As a result, smoothing constraints are applied both horizontally and vertically to the velocity model based on pre-defined correlation lengths in the tomo2d calculations (Korenaga et al., 2000). This smoothing acts to reduce the grid resolution, making it representative of the typical resolving power of travel time tomography and thereby filtering the 2D velocity model calculated from the elastic moduli estimates of the thermo-mechanical model. Tomo2d uses Gaussian smoothing within one decay length individually in the horizontal and vertical directions, based on the work of Toomey et al. (1994). In addition, when there is found to be a large residual between iterations, the inversion is repeated without outliers using a winsorisation procedure to avoid instabilities in the solution (Korenaga et al., 2000).

Smoothed p-wave velocity results from the thermo-mechanical modelling of both the purely thermal case and the melt segregation case, with inputs from table 5.1, were then compared against the velocity inversion of the travel time tomography data recorded by Paulatto et al. (2012). The comparison between the resulting velocity fields allowed for a prediction to be made of the inputs required in the thermo-mechanical model to reproduce the observed SEA-CALIPSO travel time tomography data. It was considered that there were several possible methods by which the thermo-mechanical model could reproduce the observed velocity anomaly while incorporating melt segregation, matrix compaction, and reactive flow in the system of governing equations. These include experimenting with: cooling times after intrusion, emplacement volumes, model run times, and emplacement rates.

5.3.3 Parameter testing and benchmarks

5.3.3.1 Cooling post intrusion

The first parameter tested was post-intrusion cooling time. The initial inputs were the same as in table 5.1 however the system was allowed to cool after the second set of repetitive intrusions. Sills were emplaced in two input routines over 23 ka but the system was then allowed to cool with no further sills emplaced during this time in order to allow the geotherm to relax such that crystallisation took place.

While this method aimed to keep the model inputs constant to provide a direct comparison it has a major drawback in that the total run time of the model was significantly extended. Due to the amount of melt that accumulates in high melt fraction layers in the shallow crust during melt segregation, evolution, and assimilation, the time required for cooling was much greater than the initial run time of the model.

Once the system had cooled to the point where the average melt fraction had reduced to levels similar to those inferred from field observations of erupted material from the sub-volcanic crust beneath the Soufrière Hills Volcano, the thermo-mechanical model was stopped and the outputs were converted into a smoothed velocity model using `tomo2d`. These results were then compared to the modelled and observed results of Paulatto et al. (2012). Cooling times post intrusion of 60 ka and 120 ka were investigated to give total model run times of 83 ka and 143 ka respectively.

5.3.3.2 Constant volume

The second parameter tested was model run time, in which the same total volume of melt was emplaced over a much longer time period. This has the effect of dramatically reducing the average emplacement rate of melt in the crust. The total pluton volume was kept constant in an attempt to keep the initial inputs as directly comparable as possible to those of Paulatto et al. (2012). Thickness of the intruded sills was kept the same but the time interval between sill emplacements was significantly increased. One dimensional emplacement rates of 375 mmpa, 75 mmpa, and 7.5 mmpa were investigated which are equivalent to 1/2, 1/10, and 1/100th of the rate employed by Paulatto et al. (2012) to explain the observed velocity anomaly with the purely thermal model.

5.3.3.3 Constant run time

The third parameter tested was emplacement volume. For these tests the same total model run time was used but the total volume emplaced was reduced. This has the same effect as the constant volume method in that it reduces the rate of emplacement of melt.

Due to the hypothesised existence of a double magma storage system at Montserrat it was determined that two emplacement episodes should still be used in the constant run time model. In addition, it was possible to use the updated version of the thermo-mechanical model to investigate the use of

different emplacement volumes across the two emplacement episodes. Annen et al. (2015) suggested that the intrusion rate at volcanic centres can fluctuate dramatically over the total period of growth of an intrusive igneous body, making this a credible modelling scenario.

Total pluton thicknesses of 3 km and 2.1 km were modelled using individual sills 300 m thick. For the 3 km thick pluton the first and second intrusion episodes both consisted of a 1.5 km thick zone being emplaced over the course of 2 ka with an interval of 400 years between repetitive intrusions. For the 2.1 km thick pluton the two intrusion episodes required a marginal difference in total emplaced thickness in order to maintain the 300 metre thickness of individual sills. The first intrusion episode involved 4 emplacements to total 1.2 km over 1.6 ka. The second episode of intrusions was for 3 repeated injections to total a 0.9 km thick pluton over 1.2 ka. In both instances, the interval time between emplacement episodes was increased in order to maintain the total model run time of 23 ka used by Paulatto et al. (2012).

5.3.3.4 Minimum emplacement rate

Finally, the minimum emplacement rate during melt segregation was determined that would produce the same velocity anomaly as that observed at the Soufrière Hills Volcano. Both the emplaced volume of melt and the time frame over which melt was emplaced were varied to try and match the predicted melt fractions and temperatures of Paulatto et al. (2012). Unlike the previous three methods this approach required adapting a number of the input variables. One dimensional rates of emplacement <75 mmpa were investigated using a variety of sill thicknesses to investigate the dependence of the final melt distribution on both average emplacement rate and the volume of individual emplacements. Emplacement rates used corresponded to rates at less than a tenth of that used by Paulatto et al. (2012), with emphasis on the use of 10 mmpa which fits with estimated emplacement rates in DCHZs and shallower reservoirs (Coleman et al., 2004; Solano, 2011).

Modifications were made not only to the thickness of the emplaced sills, which was reduced to 100 metres, but also to the time interval between emplacements so as to reduce the emplacement rate even further while maintaining an efficient grid spacing of 15 metres. The time step was maintained at a tenth of the CFL condition. In addition, a number of scenarios with initial sill melt fractions higher than 0.35 were used to explore how this parameter affected the ability of the thermo-mechanical model to reproduce the final velocity anomaly recovered at Montserrat.

5.4 Results

Figure 5.5 shows the comparison between the velocity anomaly from the SEA-CALIPSO seismic experiment by Paulatto et al. (2012), the results of the inversion from their purely thermal model, and those of the thermo-mechanical model when only heat diffusion is accounted for, hereafter referred to as the static model. The velocity anomaly shown in figure 5.5a is the difference between the recovered velocity model and background reference velocity of Paulatto et al. (2012). The low velocity anomaly is approximately 4 km wide directly beneath the Soufrière Hills Volcano between 6 - 9 km depth and has a maximum value of -0.7 kms^{-1} (Annen et al., 2014). There is a positive velocity anomaly immediately below the surface between 0 - 2 km depth which has been associated with the presence of lava domes and cooled intrusions (Paulatto et al., 2012; Annen et al., 2014).

The velocity anomaly shown in figure 5.5b from Paulatto et al. (2012), is generated using a multiple sill intrusion model with velocities obtained from the conversion of the modelled temperatures and melt fractions into elastic moduli data. Corresponding smoothed values, that represent the velocity anomaly that would be expected to be recovered using travel-time tomography, are shown in figure 5.5c and can be seen to produce a much lower absolute value for the large negative velocity anomaly between 6 - 9 km depth. The match between the smoothed velocity anomaly in figure 5.5c and the recovered velocity model in figure 5.5a is quite good. Figure 5.5d shows the velocity profile calculated from the elastic moduli estimations derived from the temperature and melt fraction distribution results of the thermo-mechanical model when the melt segregation terms in the governing equations are turned off. It is clear from figure 5.5d that the location of the low velocity anomaly in this static simulation run by the thermo-mechanical model is comparable to that seen in the original travel-time tomographic model.

Figure 5.5e and f show the velocity anomaly associated with a low-frequency approximation to the solution for melt distribution for the original and smoothed results respectively. Comparing figures 5.5b and e, and figures 5.5c and f shows that the thermo-mechanical model is capable of broadly reproducing the results of the purely thermal model used by Paulatto et al. (2012) to a high standard when the same inputs are used. The large low velocity anomaly can be seen at 6 - 9 km depth in both sets of modelled results and smoothing has reduced the absolute value of the velocity anomaly to approximately -0.5 kms^{-1} in the interpolation for the tomo2d inversion software. It is apparent that the smoothing method used by Paulatto et al. (2012) resulted in a stronger vertical smearing effect in comparison with the results interpolated for tomo2d. Paulatto et al. (2012) used a depth

dependent Gaussian filter which had a width equal to the approximate Fresnel radius for a signal with a dominant frequency range of 6 - 25 Hz. The difference in smoothing techniques and the vertical smearing in Paulatto et al. (2012) has resulted in a narrower velocity anomaly for the final result of the purely thermal model in comparison to that of the thermo-mechanical model.

Figure 5.6 shows the stark contrast between the results of the purely thermal model and the thermo-mechanical model when the same initial parameters are used and melt segregation is allowed to occur in the thermo-mechanical model. Panels a), b), and c) in figure 5.6 are the same results from Paulatto et al. (2012) that were shown in figure 5.5 and are included here for direct comparison. Figure 5.6d is the resultant velocity profile from the thermo-mechanical model when melt segregation is accounted for and all other parameters are kept the same as in figure 5.5d. The results produce a much stronger negative velocity anomaly, as can be seen in panel e) where the scale has been modified, with a significantly different geometry.

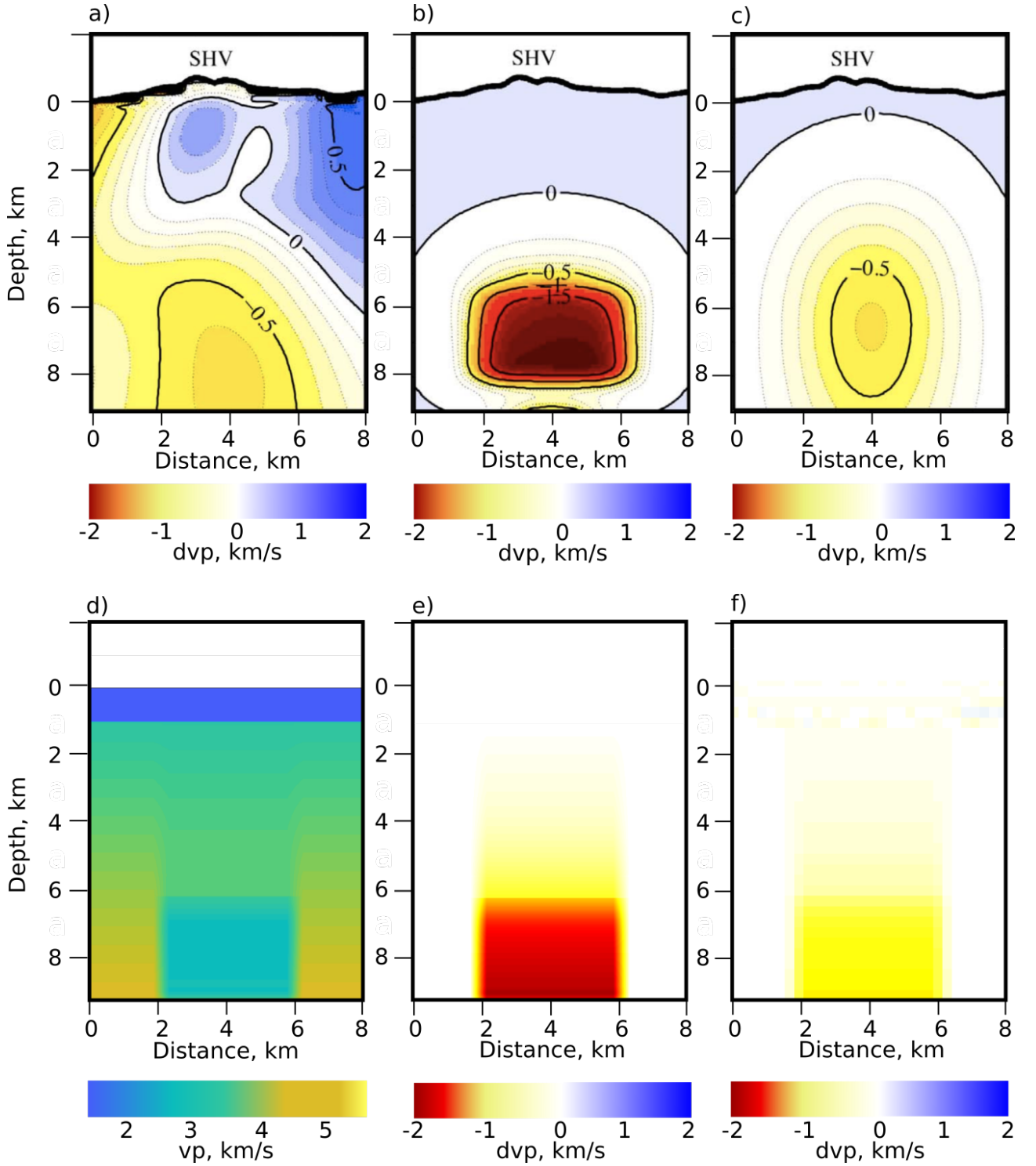


Figure 5.5: Comparison between purely thermal results of the thermo-mechanical model and those of Paulatto et al. (2012) for the velocity anomaly beneath the Soufrière Hills Volcano. a) Velocity anomaly inverted from the SEA-CALIPSO experiment by Paulatto et al. (2012), b) velocity anomaly estimated using the low-frequency approximation by Paulatto et al. (2012) from the purely thermal model, c) corresponding filtered velocity anomaly estimated by Paulatto et al. (2012), d) velocity profile calculated from the thermo-mechanical model using the static governing equations, e) corresponding velocity anomaly using the low-frequency approximation, f) re-sampled, filtered results of the velocity anomaly from the thermo-mechanical model.

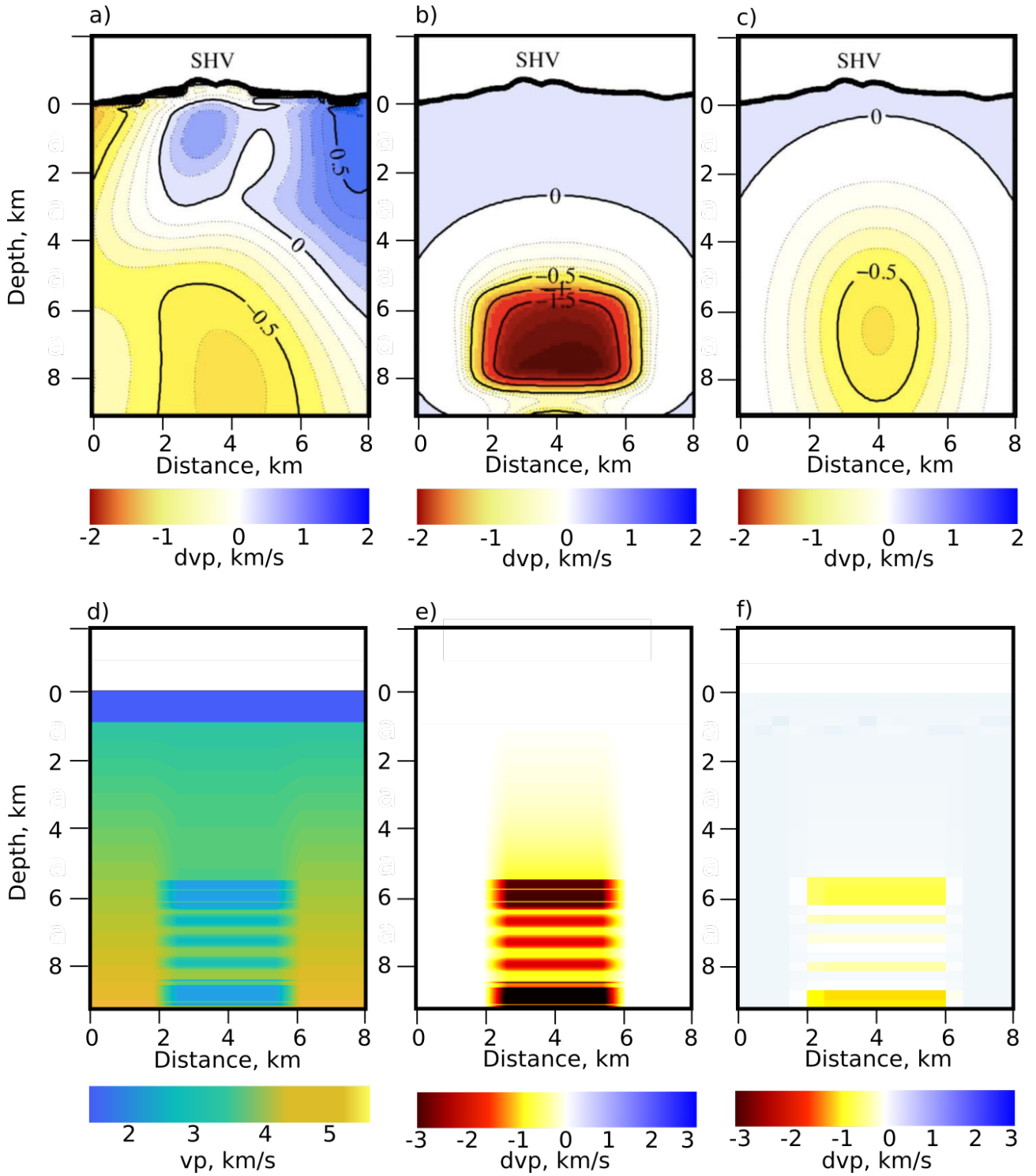


Figure 5.6: Comparison between the results of the thermo-mechanical model when melt segregation is accounted for in the solution and the results of Paulatto et al. (2012) for the velocity anomaly beneath the Soufrière Hills Volcano. a) Velocity anomaly inverted from the SEA-CALIPSO experiment by Paulatto et al. (2012), b) velocity anomaly estimated using the low-frequency approximation by Paulatto et al. (2012) from the purely thermal model, c) corresponding filtered velocity anomaly estimated by Paulatto et al. (2012), d) velocity profile calculated from the thermo-mechanical model when melt segregation, compaction, and reactive flow are accounted for in the governing equations, e) corresponding velocity anomaly using the low-frequency approximation, f) filtered results of the velocity anomaly from the thermo-mechanical model. Note difference in dvp scale for e) and f).

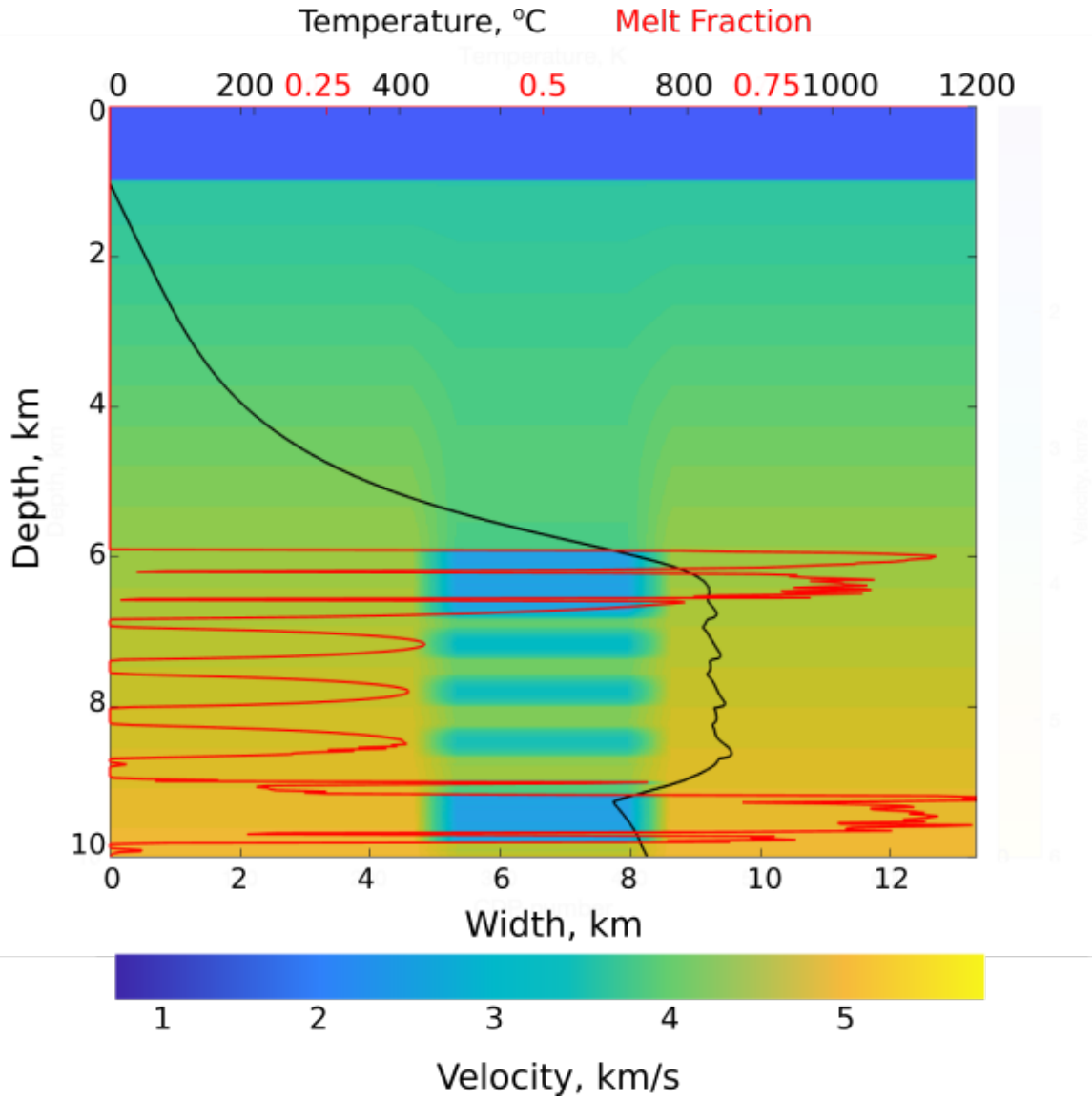


Figure 5.7: Overlay of the 1D temperature and melt fraction results over the corresponding estimated 2D velocity profile from the thermo-mechanical model using the same inputs as for figures 5.5 and 5.6 with melt segregation terms in the system of general equations turned on. The colour scale shows the range of seismic velocities in the 2D profile. The red solid line is the 1D melt fraction profile and the black solid line is the 1D temperature profile taken through the centre of the intruded pluton.

While the width of the anomaly is the same as for the static model at approximately 2 km radius, the vertical distribution is comparatively heterogeneous. Segregation of melt away from the emplaced sills into the surrounding country rock has resulted in large low velocity bands in areas of melt accumulation. This is more easily recognisable in figure 5.7 which shows a direct overlay of the 1D temperature and melt fraction results through the centre of the intrusion zone on the 2D velocity profile. It can be seen that the locations of high melt fraction correspond with the regions of the

the lowest seismic velocities in the high-resolution 2D p-wave velocity profile. Individual layers in the centre of the model with melt fractions of 0.3 - 0.35 can be seen to have significantly reduced the seismic velocities from the background gradient by almost 2.5 km^{-1} .

Unlike the static thermal model, figure 5.6 has a very low velocity zone at the base of the second emplacement region at 9 km. This large negative velocity anomaly does not correspond with a region of high temperatures in figure 5.7 as would be the case in the purely thermal model. In fact, the temperature in this region is lower than in the surrounding crust. The temperature profile shows a decoupling of the location of highest melt fraction and the location of highest temperature in the bottom half of the model. At the top of the model it is also evident that melt has accumulated above 6 km but is bounded by the location of the solidus for the country rock which is 700°C .

Smoothing the results of the thermo-mechanical model using *tomo2d* produces a reduced velocity anomaly as can be seen in figure 5.6f. The two low velocity zones at 6 and 9 km are still easily identifiable however the magnitude of each low velocity zone is approximately half that in panel e). The individual low velocity layers in the centre of the model demarcated by melt accumulation are also less apparent. While it is clear that there is a low velocity region with a negative velocity anomaly between -0.5 - -2.0 km s^{-1} , the zone is broader than in the high resolution model and more uniform.

It is clear that there is a significant difference between the velocity anomaly calculated from the SEA-CALIPSO data and the filtered result for the *tomo2d* tomography software on the velocity profile calculated from the thermo-mechanical model. This suggests that when melt segregation, matrix compaction, reactive flow, and melt evolution are taken into consideration, a different emplacement history would be required to explain the velocity anomalies beneath Montserrat.

5.4.1 Cooling post intrusion

The 1D profiles in figures 5.8 and 5.9 show the bulk modulus and estimated velocities resulting from the calculation of temperature and melt fraction using the thermo-mechanical model. In this instance the initial parameters were kept the same as in table 5.1 but melt segregation was accounted for in the equations. In addition, the system was allowed to cool following the final sill emplacement at 23 ka for time periods of 60 ka and 120 ka respectively.

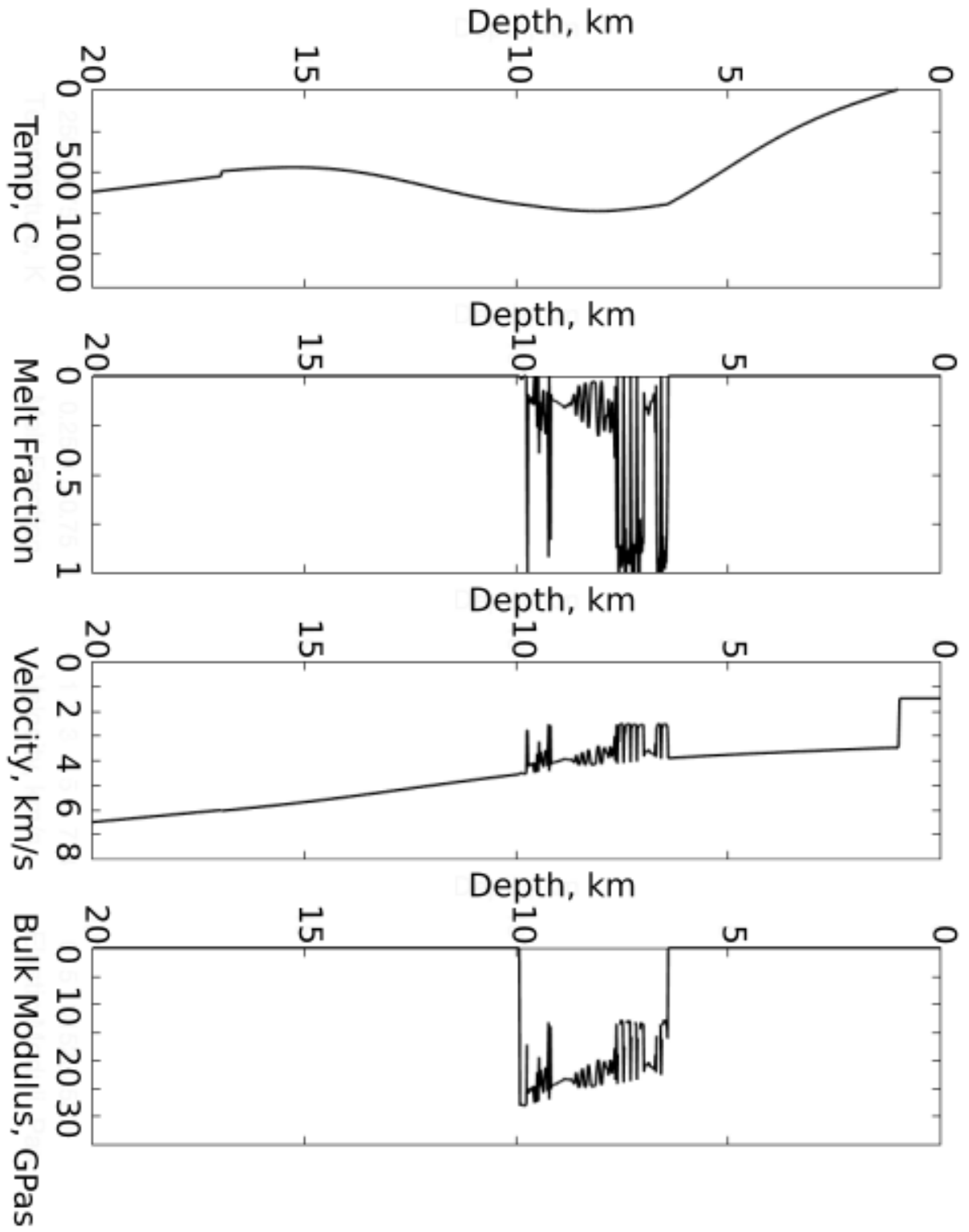


Figure 5.8: P-wave velocities resulting from the 1D temperature and melt fraction results of the thermo-mechanical model with melt segregation. The low frequency approximation to the elastic moduli calculation was used. Two sets of emplacement routines occurred with an interval of 15 ka. Both sets of repetitive emplacements were for 10 individual 300m thick sills intruded every 400 years under accretion. The system cooled for 60 ka after the final sill was emplaced.

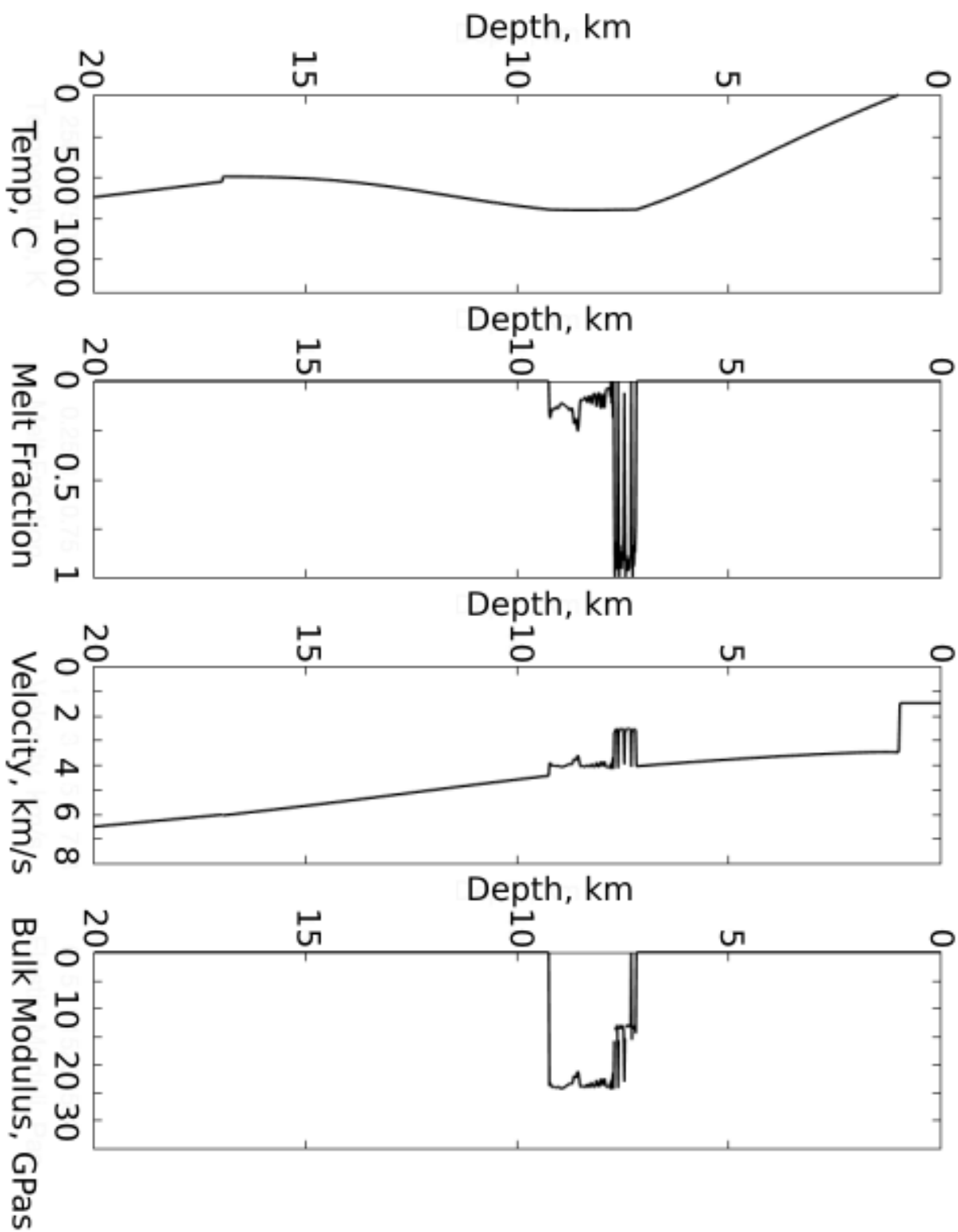


Figure 5.9: P-wave velocities resulting from the 1D temperature and melt fraction results of the thermo-mechanical model where melt segregation was taken into account during the numerical simulation. The high frequency approximation to the elastic moduli calculation was used. Two sets of emplacement routines occurred with an interval of 15 ka. Both sets of repetitive emplacements were for 10 individual 300m thick sills intruded every 400 years via under accretion. The system cooled for 120 ka after the final sill was emplaced.

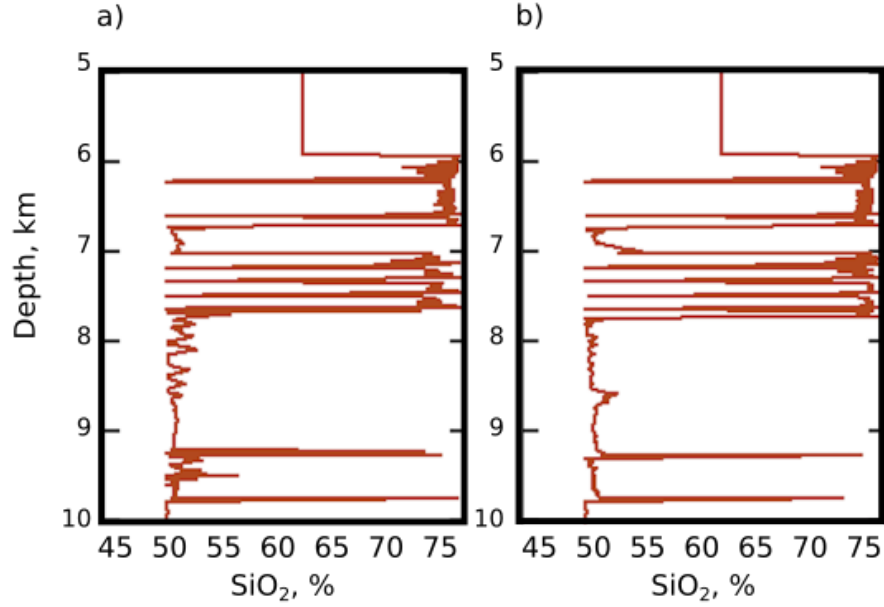


Figure 5.10: 1D silica content results through the centre of the pluton when initial parameters of the thermo-mechanical model are the same as for figures 5.6 after cooling for a) 60 ka and b) 120 ka following the final sill emplacement.

There is a clear correlation between the calculated velocities and estimated bulk modulus values in both figures. While both temperature profiles are largely smooth, there is a distinct difference in the melt fraction profiles between figures 5.8 and 5.9. Both 1D melt fraction profiles show a lot of variation throughout the system which is due to evolution of the melt composition over time as it segregates and as the system cools, and resulting changes in local silica content, shown in figure 5.10. The steep boundaries between regions of high and low melt fraction create sharp gradients in seismic velocity which can be difficult to image using geophysical techniques.

The longer cooling time in figure 5.9 has evidently resulted in relaxation of the temperature gradient and a reduction in total melt volume. Lower overall temperatures in figure 5.9 have resulted in cooling below the country rock solidus temperature at the base of the model resulting in solidification below 9 km. The largest negative velocity anomaly is marginally smaller after 120 ka in comparison to only 60 ka of cooling but is still almost twice as large as that seen in Paulatto et al. (2012) of only -0.5 km s^{-1} .

Distribution of silica appears to be fairly similar between both figure 5.10a and b, with 75% SiO_2 in the main region of melt accumulation at the top of both of the models. The melt has accumulated in this region to produce a large melt lens via segregation. At the base of the emplacement zone between 8 - 10 km, average levels of silica are marginally higher in figure 5.10a after only 60 ka of cooling. The main difference between the two models at this depth is the lack of melt in the region after prolonged cooling. Evolution of the melt results in sustained high melt fraction lenses at the locations of high silica content at 9.2 and 9.8 km depth, as can be seen in figures 5.8 and 5.10. The presence of deep melt lenses was not identified in the tomographic velocity models across Montserrat by Paulatto et al. (2012), although, if they did exist, they may have been too small to have been detected (Byerly et al., 2010).

The lowest velocity in figure 5.9 is only 2.50 km^{-1} and occurs in the regions where melt fraction is at unity. This is very evident from the 2D velocity profiles and velocity anomalies shown in figure 5.11. The 2D velocity profiles for both 60 ka and 120 ka of cooling following the final sill emplacement have been plotted, overlain by the 1D temperature and melt fraction results from the centre of the pluton in figure 5.11a and d respectively. Panels b) and e) show the velocity anomaly for the high-resolution grid from the thermo-mechanical model while panels c) and f) are the smooth inverted results from the tomo2d tomographic package.

While both cooling periods of 60 ka and 120 ka produce anomalies that are closer in style to that seen in figure 5.5 in comparison with the segregation example that only ran for 23 ka (figure 5.6, neither are able to reproduce the anomaly recorded by the SEA-CALIPSO seismic experiment. The absolute value of the velocity anomaly is simply too high across the large low velocity zone, both in the high-resolution 2D profile calculated from the results of the thermo-mechanical model and in the results following filtering. Even when the system is allowed to cool for a long period of time at 120 ka and the result is smoothed using the course grid spacing interpolation required for the tomo2d package (figure 5.11f) the large anomaly seen at the top of the emplacement zone is over four times larger (-2.4 km s^{-1}) than that of the smoothed model shown in figure 5.5.

The broad zone over which the anomaly exists in figure 5.11b and e is much wider and has a larger vertical extent despite the cooling time than in figure 5.5. The high melt fractions shown in figures 5.8 and 5.9 persist over these short time scales as the temperature gradient has not had sufficient time to relax. Longer episodes of cooling were not tested due to the time scales over which shallow magma emplacement and eruption cycles have been observed to have occurred historically at the Soufrière Hills Volcano.

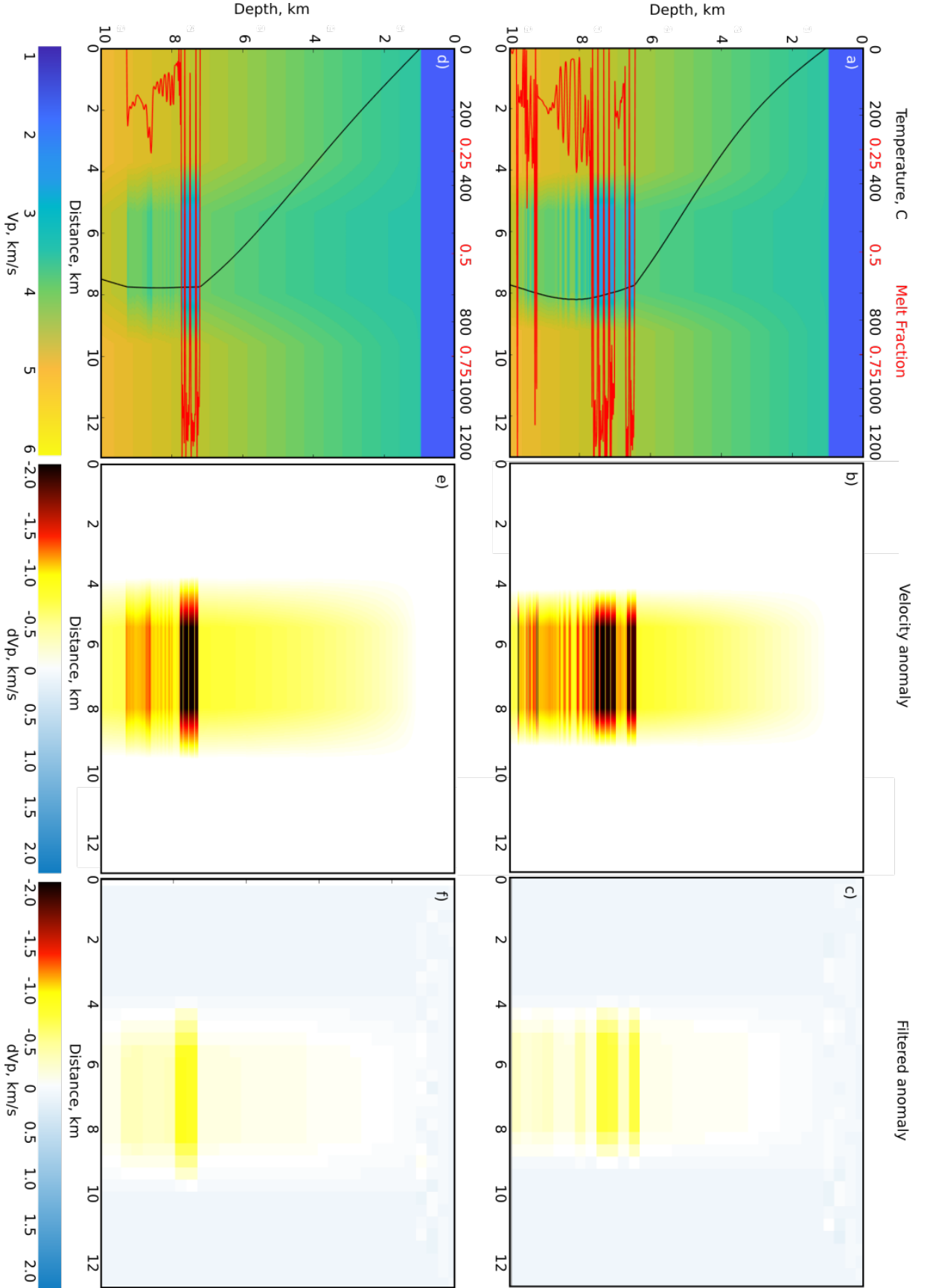


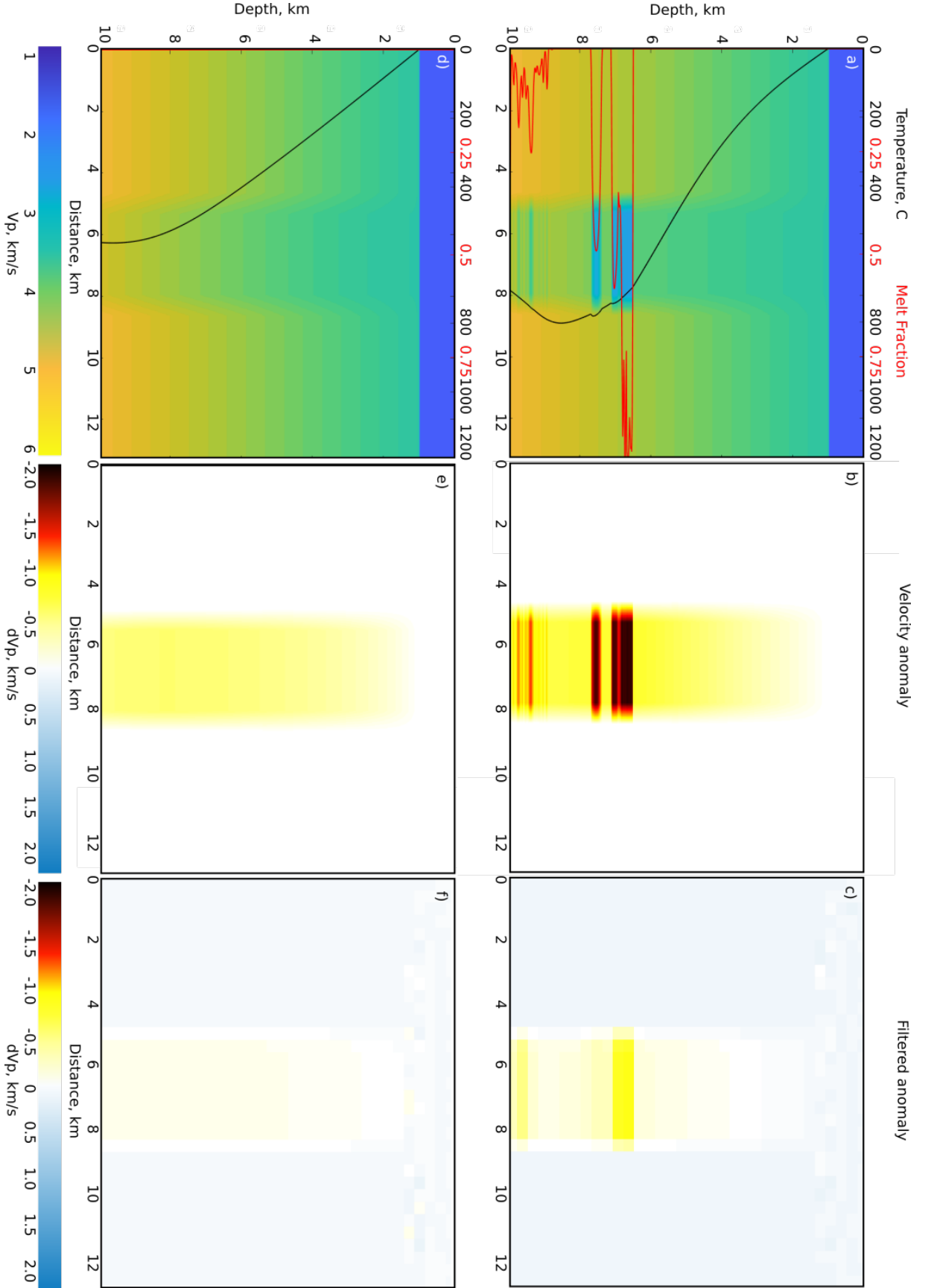
Figure 5.11: Comparison of the thermo-mechanical model results when the system is cooled for a) - c) 60 ka, and d) - f) 120 ka after the final sill emplacement. a) and d) show the 2D velocity profile with 1D melt fraction and temperatures from the centre of the domain super imposed, b) and e) are corresponding velocity anomalies, c) and f) are the velocity anomalies post filtering for tom2d software.

5.4.2 Constant volume

Figure 5.12 shows the results of maintaining the same total pluton volume as Paulatto et al. (2012) but reducing the 1D emplacement rate to 75 mmpa (panels a - c) and 7.5 mmpa (panels d - f). The thickness of emplaced sills was maintained at 300m but the time between emplacements was increased ten-fold and one hundred-fold respectively. An emplacement rate of 375 mmpa was also tested but results have not been shown as it is clear from 5.12b that the velocity anomaly would be too large to match the observed anomaly at the Soufrière Hills Volcano.

It is clear from figure 5.12a that the significant reduction in emplacement rate from 750 mmpa in Paulatto et al. (2012) to 75 mmpa is not sufficient to reduce the maximum melt fraction when melt segregation occurs. Melt has still accumulated near the top of the system, bounded at 6.5 km by the location of the country rock solidus. Accumulation is so efficient during buoyant segregation of melt that a thick high melt fraction layer persists. The velocity anomaly calculated on the high resolution grid is still very large and negative, with a maximum value of -2.09 kms^{-1} due to the high melt fractions which reach unity between 6.5 - 7 km depth. The filtered anomaly recovered using the tomo2d software has a maximum value of -1.07 kms^{-1} which is twice that calculated by Paulatto et al. (2012).

The 1D profiles shown in figure 5.13 show that the bulk modulus calculated in the emplacement zone is significantly reduced in the region of high melt fraction. It is important to note however that the bulk modulus value increases sharply to 20 GPa in the highly crystalline region between the high melt fraction layers at 7 km despite the high temperatures. This behaviour can also be seen between 9 - 10 km depth where low melt fractions, <0.25 , can be seen. Despite the high crystallinity in this region the bulk modulus, and consequently the seismic velocity, is observably reduced from the background value of 26 GPa to 22 GPa despite the temperatures in the crystalline regions being high. The resulting effect on velocity is to reduce the values in these low melt fraction lenses by $<0.5 \text{ kms}^{-1}$.



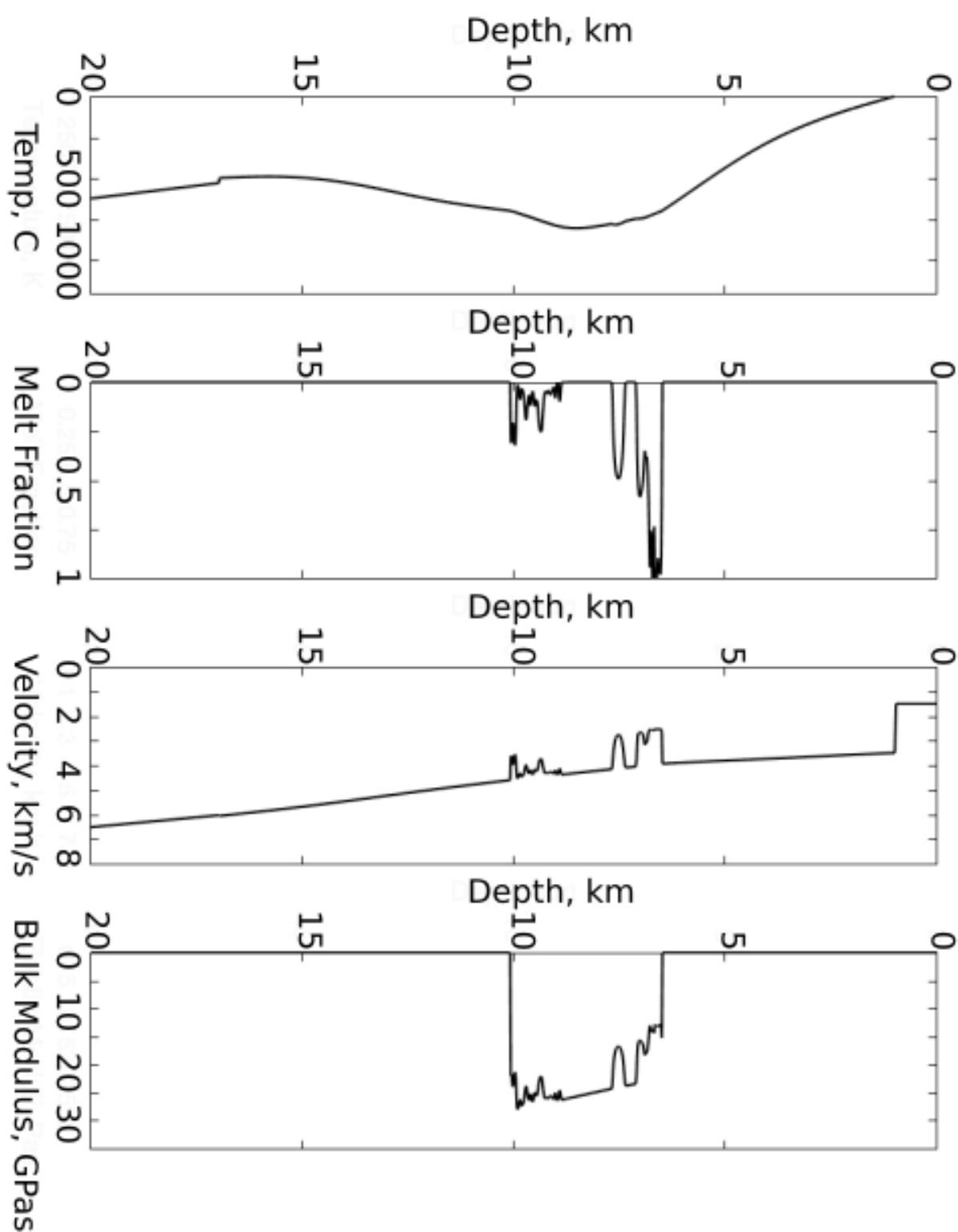


Figure 5.13: 1D temperature, melt fraction, velocity, and bulk modulus results for the same emplaced volume as in Paulatto et al. (2012) at an emplacement rate of 75 mpa.

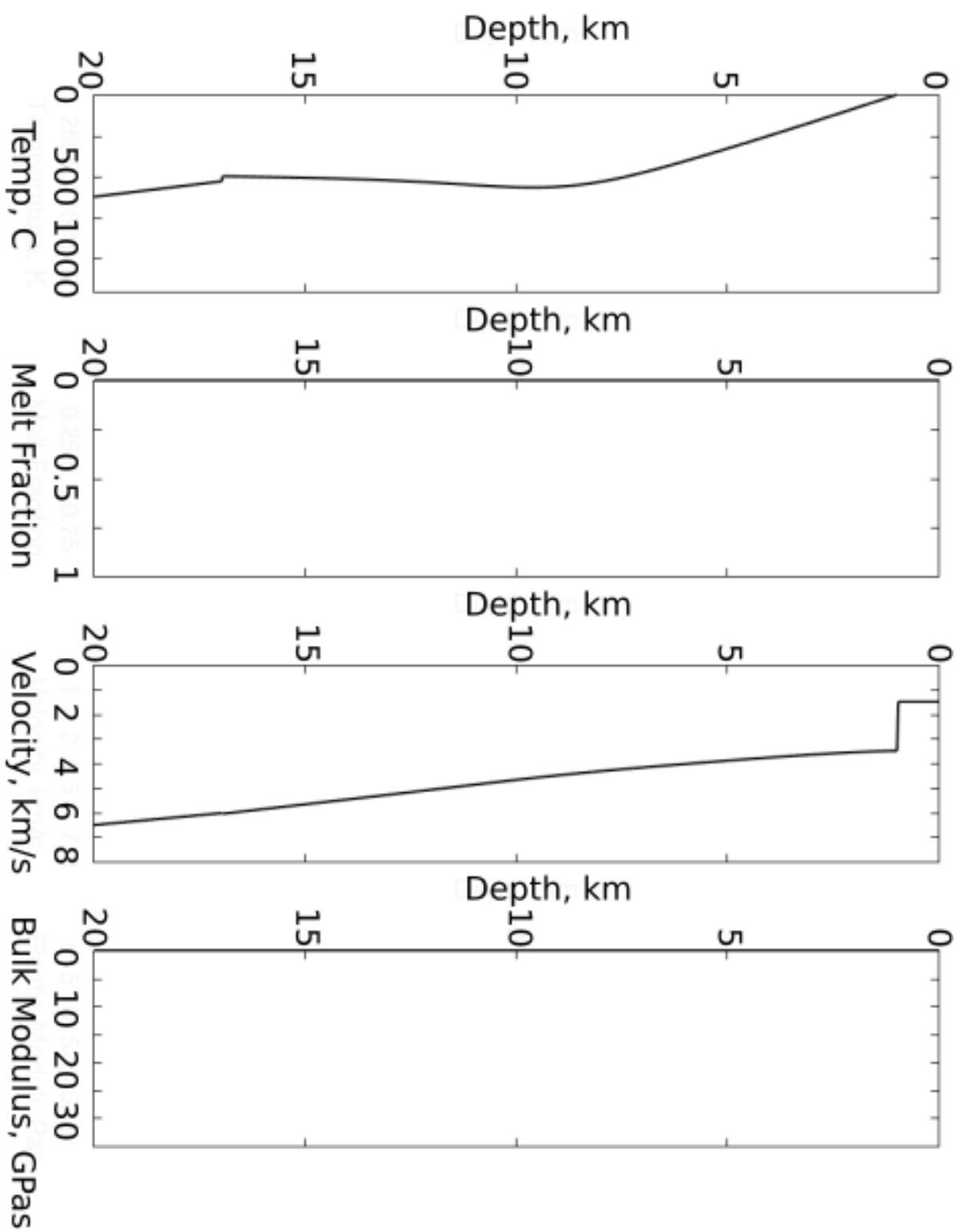


Figure 5.14: 1D temperature, melt fraction, velocity, and bulk modulus results for the same emplaced volume as in Paulatto et al. (2012) at an emplacement rate of 7.5 mpa. Incubation has not occurred and the resulting velocity profile through the emplacement zone is the same as the background velocity gradient.

Further reducing the emplacement rate to only 7.5 mmpa with 300 metre thick sills required an emplacement interval of 40 ka compared to the 400 year interval used by Paulatto et al. (2012). While the melt in individual sills evolved slightly in between repetitive emplacements, as can be seen from the variation in SiO_2 % throughout the domain corresponding to emplaced sill locations in figure 5.15, the total emplaced volume was not sufficiently incubated over the run time of 815 ka to produce a persistent melt fraction. This can be seen in figure 5.14 where the temperature and velocity profiles have relaxed back to the original background gradients despite the long duration of sill emplacements. The bulk modulus in this case has not been shown as it is only calculated in the instance where a velocity anomaly must be accounted for due to temperatures above the solidus or the presence of melt.

As a result of the cooling period and solidification between emplacements, the velocity anomaly produced in figure 5.12e is very broad and low with a maximum negative value of -0.31 kms^{-1} . This is much closer in value to the observed velocity anomaly at the Soufrière Hills Volcano of -0.5 kms^{-1} shown in Paulatto et al. (2012) however it is caused only by an increase in the background temperature of the system rather than by the presence of melt. In addition, the velocity anomaly was not able to be recovered by the travel-time tomography package tomo2d, evidenced by the lack of structure seen in figure 5.12f despite the increased temperatures in the system. The long time between emplacements when large individual sill thicknesses are modelled means that a much longer over-all model run time would be required for incubation to occur and for a persistent melt layer to form.

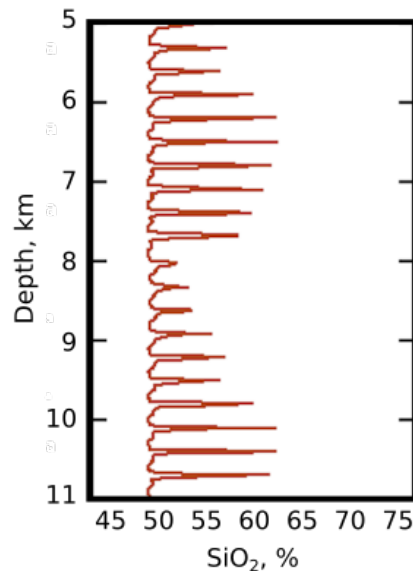


Figure 5.15: 1D silica content results through the centre of the pluton when initial parameters of the thermo-mechanical model are the same as for figure 5.6 but the emplacement rate is reduced to 7.5 mmpa by increasing the interval between emplacements of 300 metre thick sills to 40 ka.

5.4.3 Constant run time

The following results show the case where the total emplaced pluton thickness was reduced but all other parameters were kept the same as in Paulatto et al. (2012). Initial thickness of the incoming sills was maintained at 300 metres and the emplacements occurred over two intrusion episodes. The interval time between sills was kept the same at 400 years but the interval between the two intrusion episodes was increased to maintain the same total model run time of 23 ka.

Figure 5.16a - c shows the results when the total thickness of the two emplacement episodes is 3 km, half that used by Paulatto et al. (2012). In order to maintain the 300m thickness of individual intrusions at a rate of 750 mmpa and two separate emplacement episodes, the time interval between the two emplacement episodes was lengthened to 19 ka. Due to the high volume of melt being emplaced over a short time span in the second emplacement episode the residual melt from previous emplacements has not had time to fully cool. Melt has accumulated at the top of the system with a maximum melt fraction of unity at a depth of 5.97 km. The sharp contrast between high porosity layers when a total pluton volume of 3 km is emplaced results in distinct layering in both the high resolution and tomo2d recovered velocity anomalies in panels b) and c). The recovered anomaly in panel c) however is missing a great deal of structure, particularly between 7 - 8 km where there are two thin lenses in which melt fraction reaches 0.25, separated by a slightly more crystalline layer. The lenses in this instance are too narrow to be differentiated by the travel-time tomography and so produce an anomaly with a maximum negative value of -0.7 kms^{-1} . The melt fractions are much higher than those calculated in the thermal modelling of Paulatto et al. (2012), resulting in a final filtered velocity anomaly with a maximum amplitude more than twice the size of that observed at the Soufrière Hills Volcano of -1.15 kms^{-1} .

Reducing the total emplaced pluton thickness further to only 2 km, a third of the thickness used by Paulatto et al. (2012), produces still less pronounced layers, particularly after smoothing was applied (4.14f), where only one low velocity layer is recovered using tomo2d. The maximum negative velocity anomaly in panel f) is -0.8 kms^{-1} which is still significantly larger than that observed at the Soufrière Hills Volcano. The significant reduction in melt fraction seen in figure 5.16 panel d), to a maximum value of only 0.51 at 6 km, produces a total melt fraction and temperature signature with a corresponding velocity anomaly more similar to that detected by the SEA-CALIPSO seismic experiment. 1D results for temperature, melt fraction, p-wave velocity, and bulk modulus are shown for the case of a 2 km thick intruded pluton in figure 5.17.

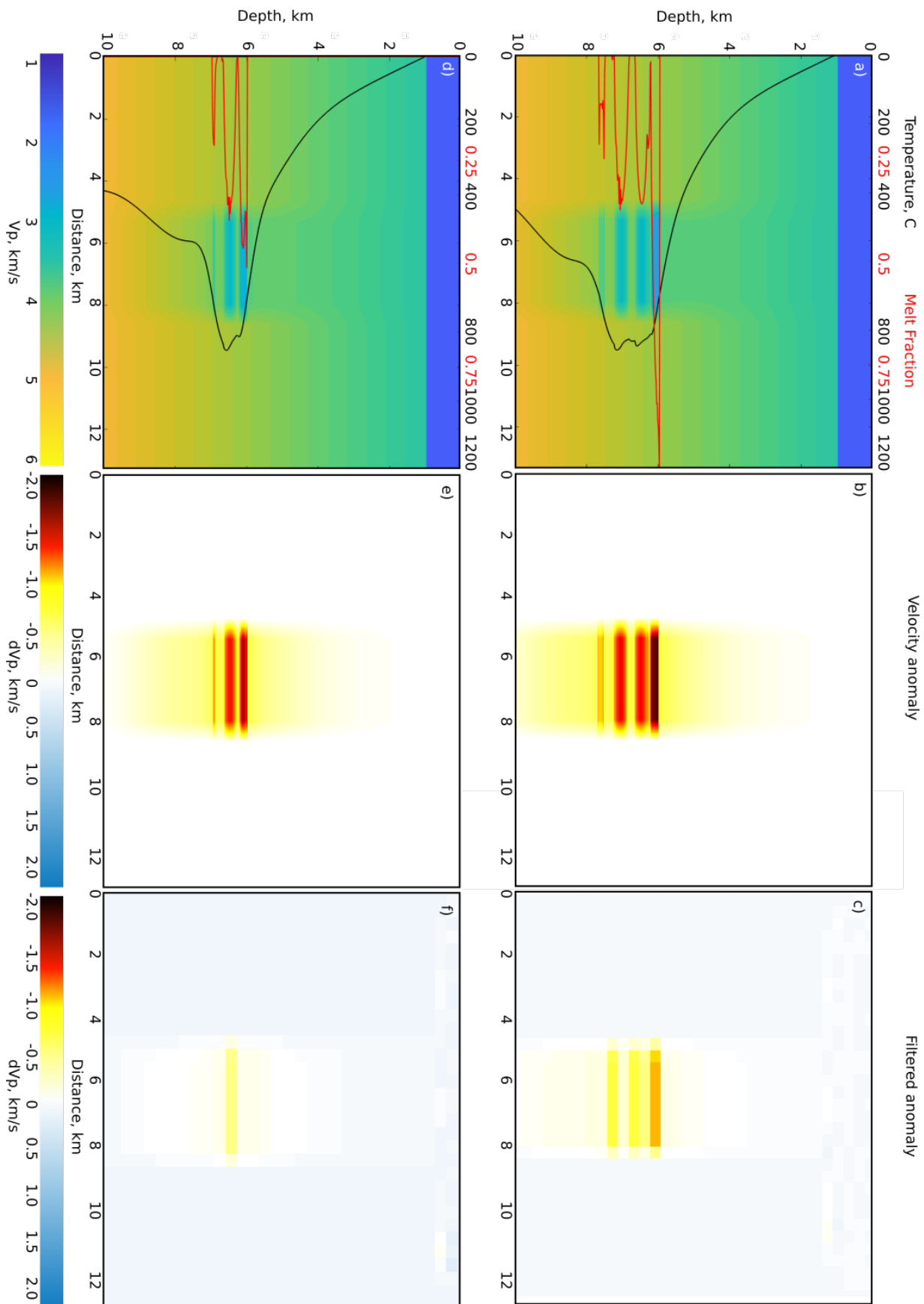


Figure 5.16: Comparison of thermo-mechanical results for total emplaced thicknesses of a) - c) 3 km, and d) - f) 2 km, with the total run time staying the same as in Paulatto et al. (2012). a) and d) show the 2D velocity profile with 1D melt fraction and temperatures super imposed, b) and e) are corresponding velocity anomalies, c) and f) are the anomalies post filtering using `tomod2d`.

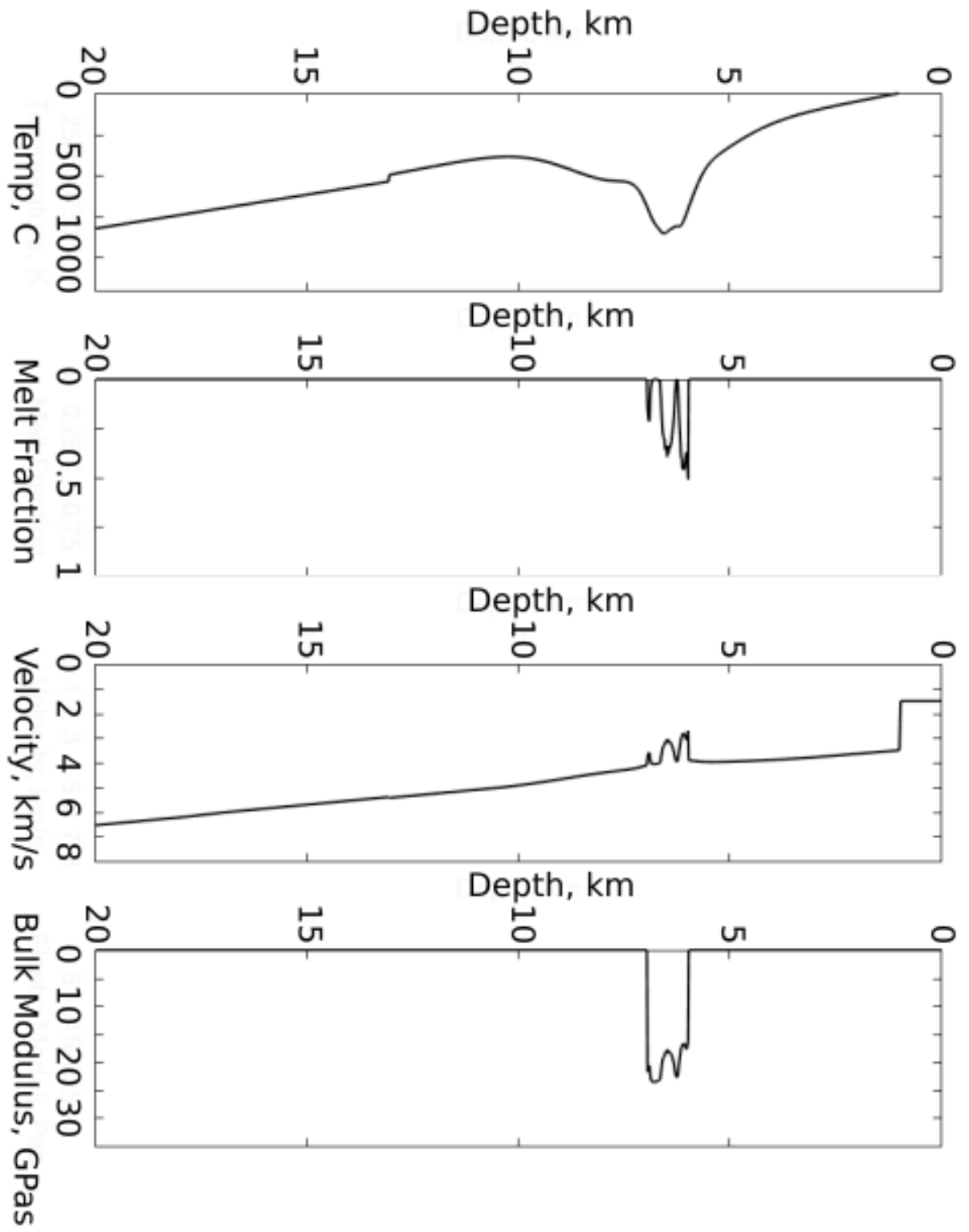


Figure 5.17: 1D thermo-mechanical results for a total emplaced thickness of 2 km, with the total run time staying the same as in Paulatto et al. (2012). a) shows the 1D temperature profile, b) is 1D melt fraction, c) is the 1D velocity profile, and d) is the 1D bulk modulus values through the centre of the pluton relating to figure 4.16d-f.

The clear correlation between reduction in bulk modulus with the presence of melt can be seen in the 1D profiles. The dependence of seismic velocity on crystallinity is very apparent from the increase in velocity in regions where melt fraction reduces to zero due to compaction despite temperatures being maintained well above the solidus. At 6.5 km depth the bulk modulus remains high at 18 GPa in between the high melt fraction layers.

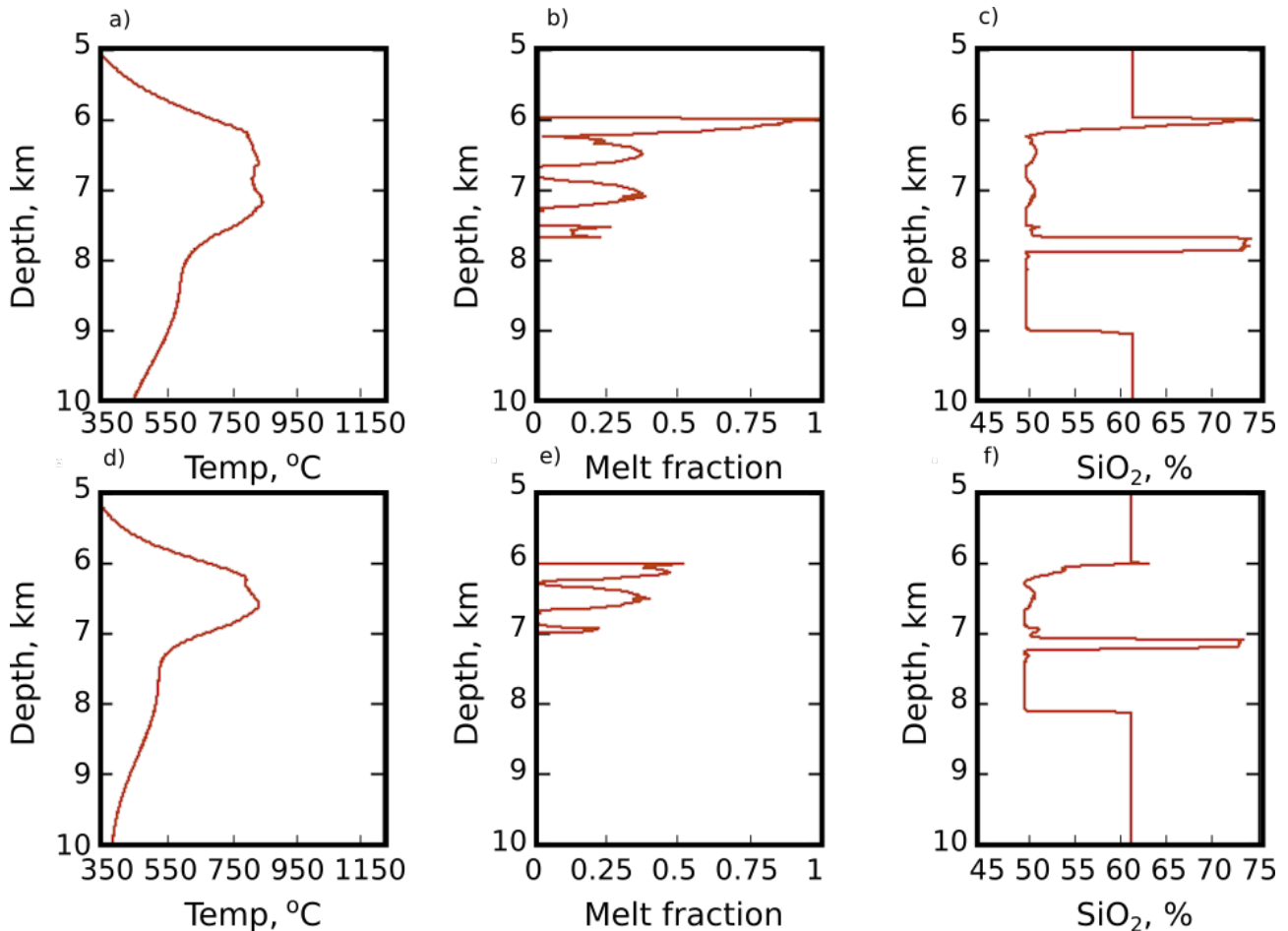


Figure 5.18: 1D temperature, melt fraction, and silica content results through the centre of the pluton when initial parameters of the thermo-mechanical model are the same as for figure 5.6 but the total thickness of emplaced plutons are a) - c) 3 km and d) - f) 2.1 km.

Figure 5.18 shows the 1D temperature, melt fraction, and SiO₂ % results for a) - c) 3 km total emplaced volume and d) - f) 2.1 km total pluton thickness. It is clear from the melt fraction comparison (b) and e)) that the difference in total emplaced volume has resulted in a significant difference in the maximum melt fraction values at the top of the system. The reduction in total pluton thickness to only 2.1 km produces a lower maximum melt fraction value after 23 ka and therefore a signature that is more similar to the purely thermal modelling results. The SiO₂ % results show a large spike in the concentration to 73.5% at the base of the emplaced plutons where the compacting boundary is found

and the melt fraction is zero. There is a significant increase in SiO_2 concentration at the top of the system in figure 5.18c where the larger total intruded volume of melt has resulted in accumulation of melt at the top of the system.

5.4.4 Minimum emplacement rate

In sections 5.4.1 - 5.4.3 the initial parameters of the thermo-mechanical modelling were kept as close as possible to those of Paulatto et al. (2012) and only one variable was changed at a time in order to explore the sensitivity of the results to that variable. In contrast, the simulations shown in this section deviate from the initial model inputs across a number of parameters simultaneously. This was done to try to find the lowest possible emplacement rate at which the observed seismic velocity anomaly at the Soufrière Hills Volcano could be reproduced when segregation and reactive flow were included in the modelling process.

Figure 5.19 shows the results when 100 metre thick sills were emplaced at a) - c) 5 km below the sea floor, and d) - f) 3 km initial emplacement depth. The 1D emplacement rate used was 10 mmpa with two emplacement episodes separated by 15 ka to give a total emplaced thickness of 6 km over a time frame of 0.615 Ma. All other initial model parameters describing the properties of the country and intruding rock types were maintained the same as those used by Paulatto et al. (2012) in their static model.

While previous results using reduced emplacement rates were unable to reduce the maximum melt fraction while maintaining a large low velocity zone, figure 5.19a shows that the maximum melt fraction in this scenario is only 0.41. This matches closely with the maximum estimated melt fraction determined by Paulatto et al. (2012) from the observed SEA-CALIPSO seismic survey beneath Montserrat. The melt fraction varies with depth and a distinction can be seen between the first and second emplacement batches at a depth of 8.8 km. The use of thinner intruding sills in comparison with previous attempts of the thermo-mechanical and static models to reproduce the observed velocity anomaly has resulted in thinner high fraction melt lenses interspersed with more crystal-rich regions as opposed to the porosity waves seen in previous results such as figure 5.16 where average melt fractions were a lot higher and the melt lenses were thicker. The difference in thickness of the low velocity regions between figures 5.16 and 5.19 is most likely a factor of the difference in run time for the two scenarios. The longer total model run time in figure 5.19 provides a longer time for diffusion to occur and therefore results in a lower overall crystal fraction and thinner melt lenses.

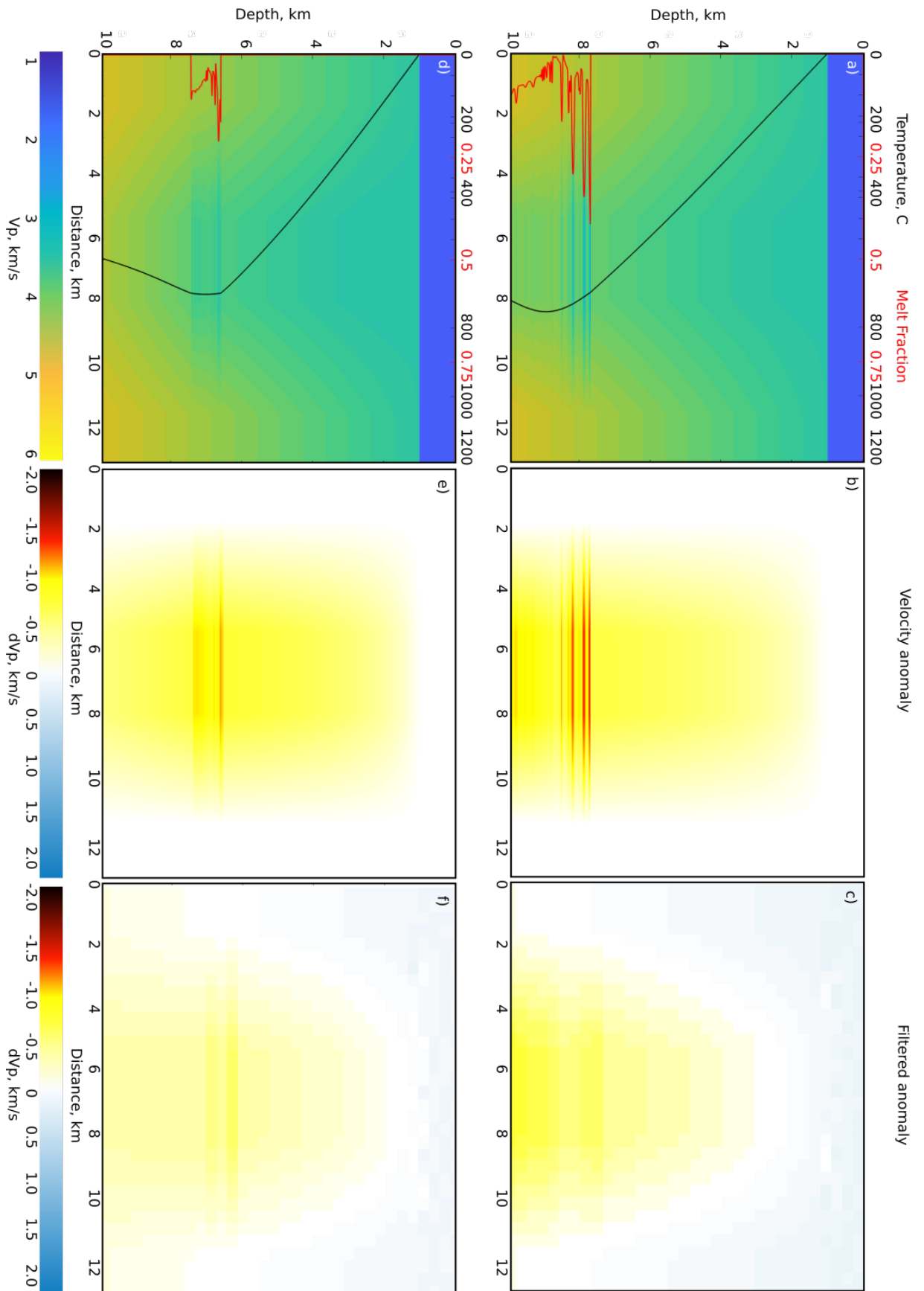


Figure 5.19: Comparison of thermo-mechanical results for sills 100 metres thick emplaced at 10 mmpa at 5 km and 3 km below the sea floor to give a total emplaced thickness of 6 km. a) and d) show the 2D velocity profile with 1D melt fraction and temperatures super imposed, b) and e) are corresponding velocity anomalies, c) and f) are the anomalies post filtering using `tomod`.

In addition, the velocity anomaly shown in panel b of figure 5.19 shows a much larger horizontal and vertical extent than those of either figures 5.12 or 5.16. This is due to the diffusion of heat over the long emplacement time from the many individual sills. Filtering the velocity anomaly in figure 5.19c using `tomo2d` has a much reduced effect compared to previous examples of smoothing. While three distinct melt lenses are visible in panel b, with a largest negative velocity anomaly at 7.865 km depth of -1.56 km s^{-1} , they have been smoothed in panel c to give a reduced maximum negative velocity anomaly of only -0.83 km s^{-1} . In comparison with the observed velocity anomaly at the Soufrière Hills Volcano, the synthetic anomaly produced from the thermo-mechanical model in figure 5.19b has a much deeper velocity anomaly, with the top of the low velocity zone marked by the shallowest melt lens at 7.685 km. The unfiltered results show a deeper broad anomaly averaging -0.8 km s^{-1} from 9 km depth to the base of the plotted system which correlates with the melt and temperature distributions in panel a). In addition, a very thin low velocity zone can be seen on this high resolution grid at 9.8 km with a value of -1.2 km s^{-1} . The depth of the high melt fraction region in figure 5.19a is much greater than the estimated depth at which melt exists at the Soufrière Hills Volcano due to the nature of the method of under accretion by which the melt was emplaced.

Figure 5.19d - f shows the results from the same initial input parameters but with an initial emplacement depth 3 km below the sea floor. This was tested to ascertain whether shallower initial emplacements would lead to a more similar velocity profile as that recorded by the SEA-CALIPSO seismic survey. The cooler temperatures of the surrounding country rock have resulted in lower final melt fractions and a longer incubation period. While the broad low velocity zone has a similar average value as the static model the emplacements are too shallow to produce the deeper mush column seen in panels a) - c). In addition, the final melt fractions are much lower than those observed in the thermal model. The smoothed anomaly is very similar to the final estimate for the velocity anomaly on the high-resolution grid but appears marginally shallower due to the coarse interpolation.

Finally, a simulation was run which used a shallower emplacement depth than most of the previous models of 4 km. The intrusion rate was maintained at 10 mmpa, as in figure 5.19 and sill thickness was kept at 100 metres to give the final temperature and melt fraction profiles shown in figure 5.20 superimposed on the velocity profile. The results of this run of the thermo-mechanical model were determined to show the best correlation with the recorded and modelled anomalies at Montserrat by Paulatto et al. (2012). Figure 5.21 shows the direct comparison between the SEA-CALIPSO observed velocity anomaly, the synthetic results from the purely thermal model, and the final results of the thermo-mechanical model, where emplacement has occurred at an initial depth 4 km below the sea floor. The velocity anomaly from the thermo-mechanical model has a greater vertical and horizontal

extent but both the maximum negative velocity anomaly (-1.61 km s^{-1}) in 5.21e and the maximum negative filtered anomaly from tomo2d (-0.65 km s^{-1}) in panel f) closely match the recorded values in panel a). 1D profiles for the temperature, melt fraction, velocity, and bulk modulus results for the case shown in figure 5.21 can be seen in figure 5.22. The bulk modulus values calculated in the pluton emplacement zone where melt fractions are greater than one shows the dependence of bulk modulus and consequently seismic velocity on the presence of melt. The temperature profile is very smooth and although there is a variation in temperature values throughout the emplacement region, the locations of high melt fractions can be seen to correspond with drops in bulk modulus and seismic velocity to a greater extent than changes in temperature. A comparison between the 1D temperature and melt fraction profiles through the centres of the final thermal and thermo-mechanical models is shown in figure 5.23. The temperature profile can be seen to be much smoother in the thermo-mechanical model due to the significantly increased total model run time which allows for a greater amount of diffusion and therefore sharp contrasts are no longer present.

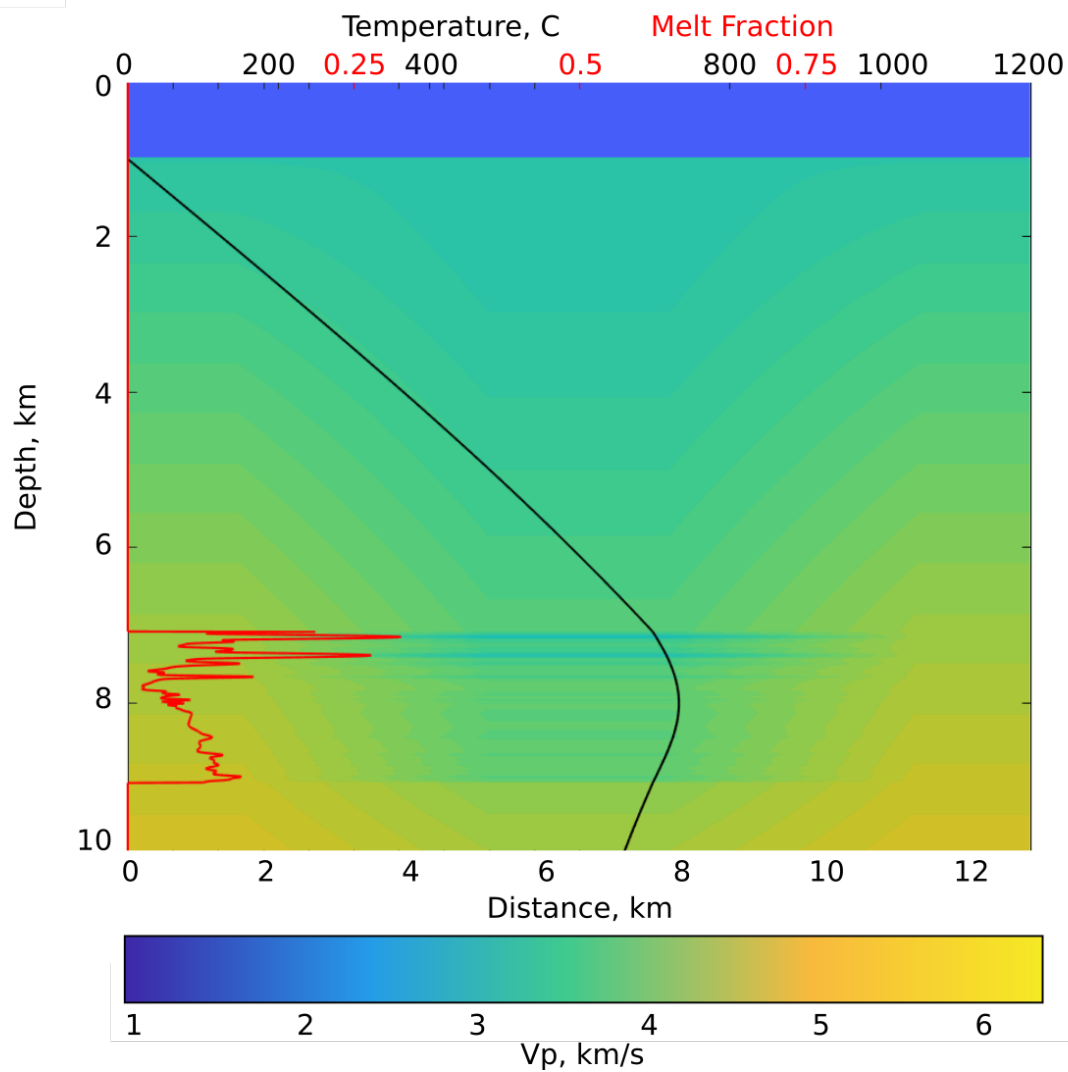


Figure 5.20: The final 1D temperature and melt fraction profiles are shown superimposed over the final 2D velocity profile for the case of 100 metre thick sills emplaced at 10 mmpa at a depth of 4 km.

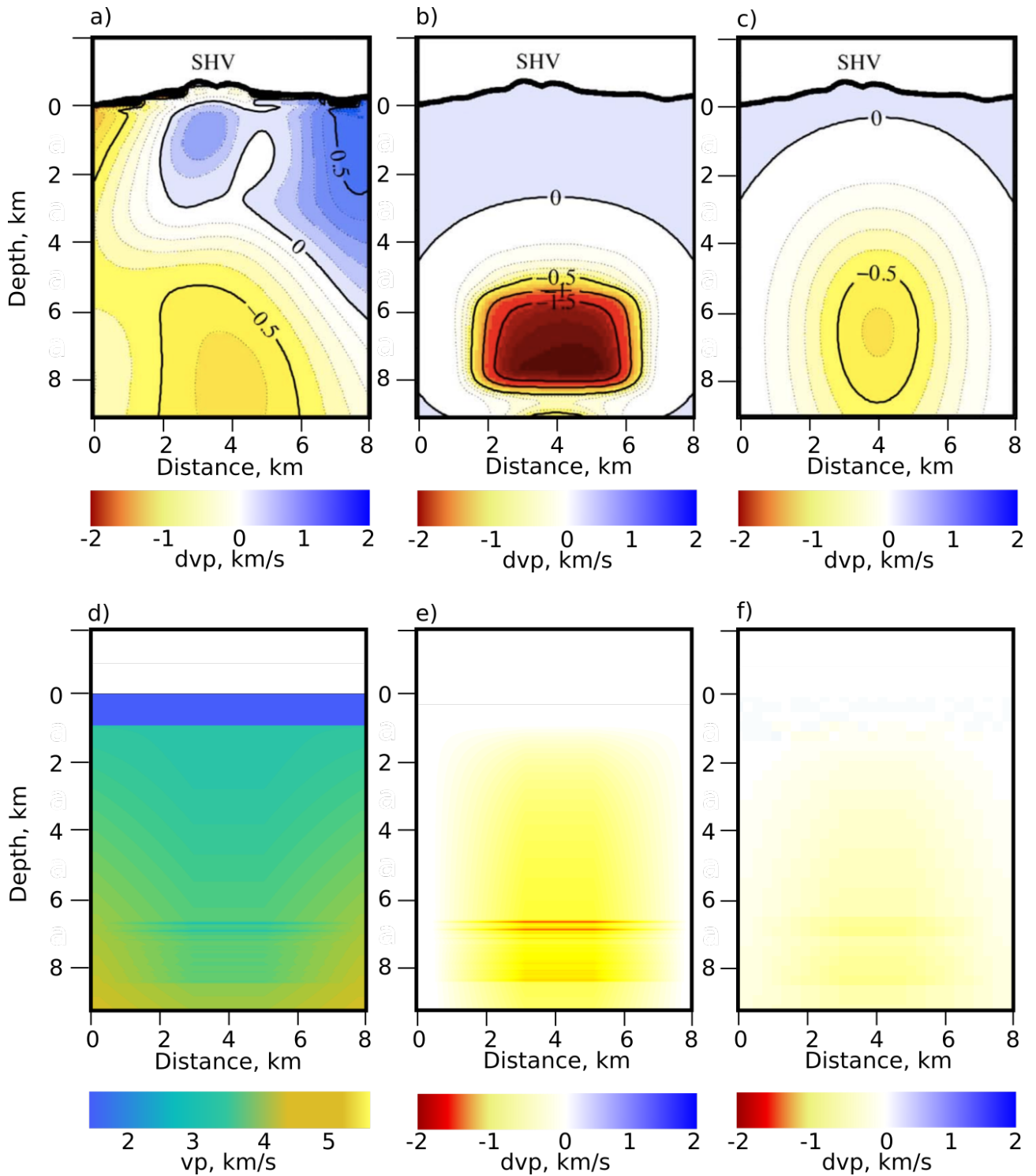


Figure 5.21: Comparison between the results of the thermo-mechanical model when melt segregation is accounted for in the solution and the results of Paulatto et al. (2012) for the velocity anomaly beneath the Soufrière Hills Volcano. a) Velocity anomaly inverted by Paulatto et al. (2012), b) velocity anomaly estimated using the low-frequency approximation by Paulatto et al. (2012) from the purely thermal model, c) corresponding filtered velocity anomaly estimated by Paulatto et al. (2012), d) velocity profile calculated from the thermo-mechanical model when melt segregation, compaction, and reactive flow are accounted for in the governing equations and initial emplacement is 4 km below the sea floor using 100 metre thick sills at 10 mmpa, e) corresponding velocity anomaly using the low-frequency approximation, f) filtered results of the velocity anomaly from the thermo-mechanical model.

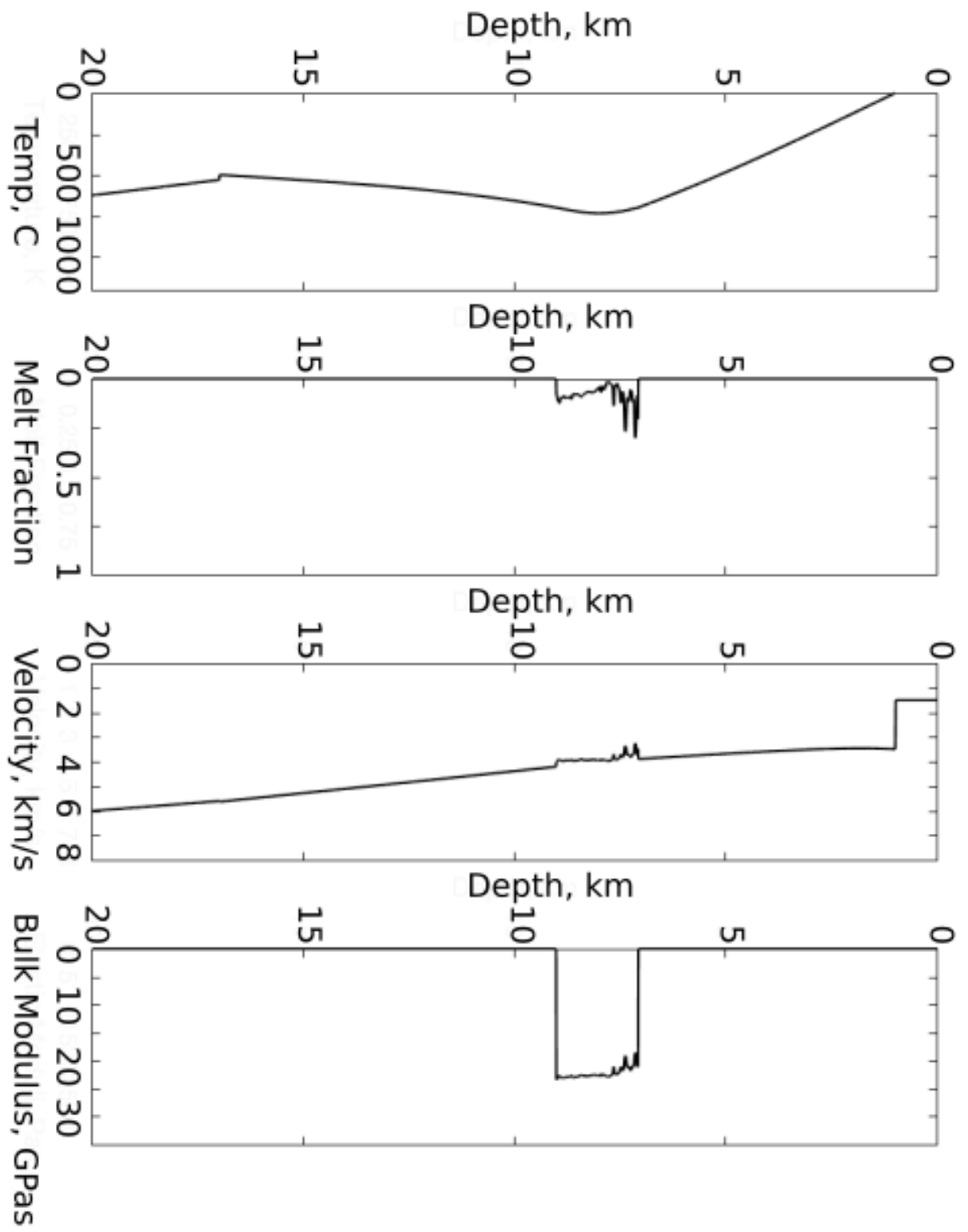


Figure 5.22: 1D temperature, melt fraction, seismic velocity, and bulk modulus results of the final thermo-mechanical model. The low frequency approximation to the elastic moduli calculation was used. 100m thick sills were emplaced at 10m for 615ka.

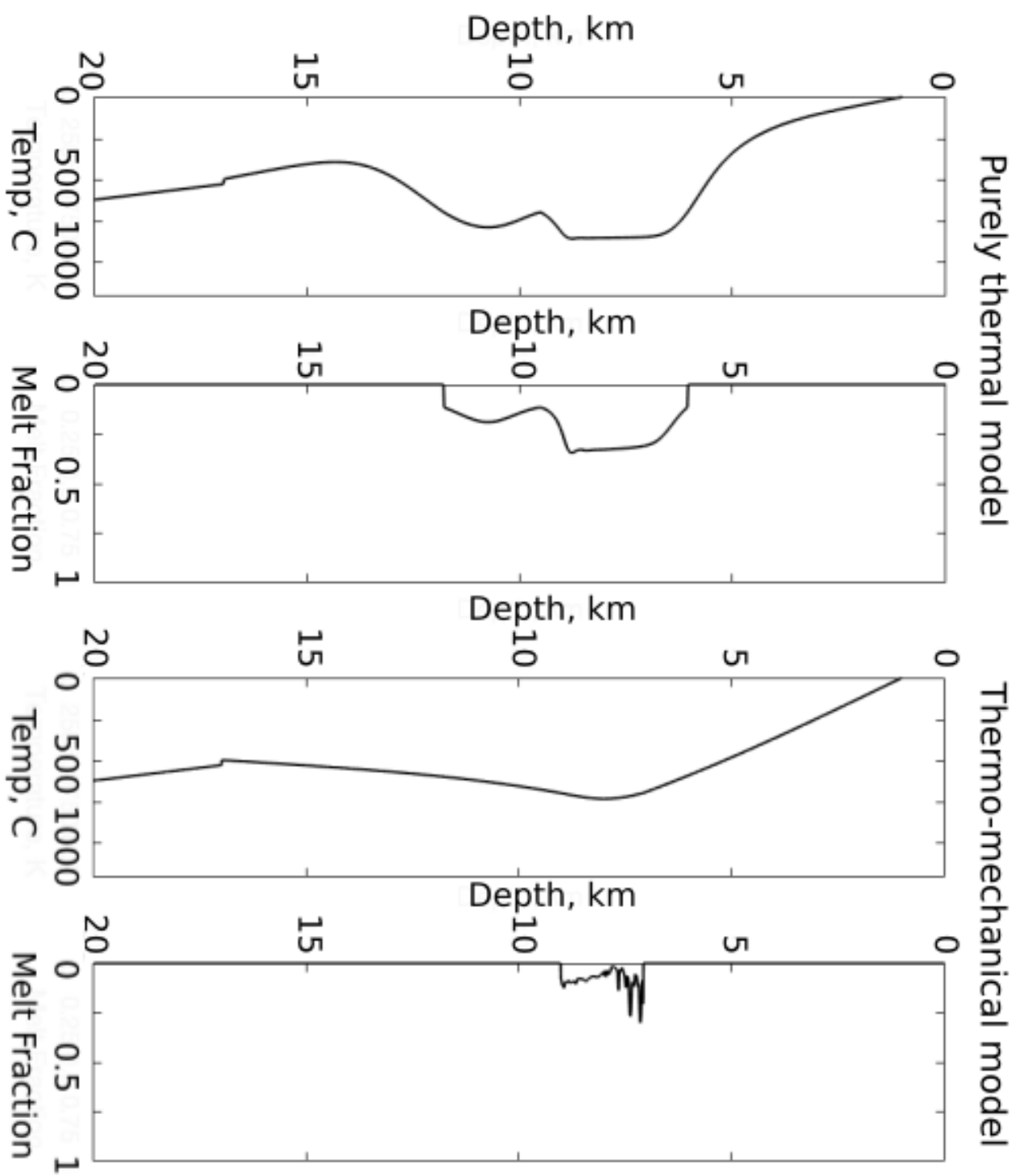


Figure 5.23: 1D temperature and melt fraction results of the purely thermal model and the thermo-mechanical model. The low frequency approximation to the elastic moduli calculation was used. Purely thermal modelling used repetitive emplacements of 300m thick sills at 750mmpa for 23ka. Thermo-mechanical modelling used 100m thick sills at 10mmpa for 615ka.

5.5 Discussion

Sections 5.4.1 - 5.4.3 show that it is quite difficult to exactly replicate the observed large negative velocity anomaly when including melt segregation in the system of governing equations. As sills are brought into the sub-volcanic system in the shallow crust in the purely thermal model they must incubate for a long period of time before a large volume of eruptible melt is able to form. In contrast, as seen in figure 5.6, the thermo-mechanical model is capable of producing much larger volumes of melt in the shallow crust at lower crystal volume fractions when the same input parameters are used. The melt is concentrated in melt lenses which are interspersed with a low melt fraction mush volume. The high melt fraction layers correspond to regions where chemical evolution has resulted in a lower solidus temperature for the melt which can therefore stay liquid at much lower temperatures.

The difficulty in replicating the observed velocity anomaly at Montserrat is due to the non-uniqueness of the problem. Multiple potential models exist that would be capable of explaining the anomaly and are dependent on the initial inputs used in the modelling process. By varying the multiple parameters of the model one at a time this work has attempted to determine a fit for the observed anomaly using a fundamental understanding of the region and its volcanic history. A qualitative 'Occam's Razor' approach was used to determine whether the results produced from different variations on the input parameters were a suitable fit to the observed seismic data. It is therefore important to note that while care has been taken to consider the likely scenarios based on knowledge of Montserrat's volcanic history and its geology, the modelled scenarios only represent a 'best fit' to the observed anomaly. The only way to determine whether either the thermo-mechanical modelling predictions or the static predictions of the evolution of the spatio-temporal distribution of melt fraction are correct would be to undertake a more detailed geophysical study on Montserrat.

Varying the model parameters one by one narrowed the wide range of potential inputs for the modelling process, thereby providing a deeper insight into the mechanics of the system and the non-uniqueness of the solution when attempting to replicate a seismic velocity anomaly using the thermo-mechanical model. Long cooling times had the desired result of lowering the absolute final velocity anomalies, such as those seen in figure 5.11 for the shallow volcanic system. However, the high melt fractions which accumulated in the porosity waves observed in figure 5.9 suggest that the melt would have been mobile with the potential for an eruption before the end of the 23 ka intrusion sequence used by Paulatto et al. (2012) in their static model, let alone after the full 120 ka of cooling had taken place. In addition, the long time scale is not consistent with the cyclical activity seen at the Soufrière Hills

Volcano in Montserrat which usually experiences activity over cycles of $10^3 - 10^4$ years. This suggests that the melt would have been evacuated from the volcanic plumbing system long before the required amount of cooling would have taken place for the melt fraction to reduce to the levels seen in figure 5.11.

Maintaining the total emplaced pluton thickness at 6 km but increasing the total run time of the model to lower the emplacement rate was similarly incapable of producing a synthetic velocity anomaly similar to the recorded anomaly observed by Paulatto et al. (2012). Reducing the emplacement rate to only 7.5 mmpa produced a velocity anomaly resulting solely from the effect of temperature. The thickness of the incoming sills, kept at 300 metres, required that the interval between emplacements be increased to 40 ka. As a result, the system did not incubate and despite the chemical evolution observed in figure 5.15, temperatures fell below the country rock solidus between emplacements and persistent melt fractions were not able to form. It is important to note from the comparison between figure 5.12b and 5.12d that the presence of melt has a much greater effect on reducing the velocity at which p-waves travel through the crust than temperature. The lack of melt in panel d) results in a broad but very low negative velocity anomaly whereas the regions of high melt fraction in panel a) show a significant decrease below 3.5 km s^{-1} in regions where the melt fraction approaches unity.

Due to the speed of melt accumulation and chemical evolution in the system, when the sill thickness was maintained and the emplacement rate was increased such that persistent high melt fractions formed, the crystallinity never reduced to match that predicted by Paulatto et al. (2012). As a result, the melt fraction signature predicted from the observed low seismic velocity zone beneath the Soufrière Hills Volcano could not be reproduced by emplacing 300 metre thick sills to form a 6 km thick pluton.

Lowering the emplacement rate by reducing the total volume of melt emplaced in the shallow crust over the 23 ka run time of the model (figure 5.16) produced pronounced porosity waves. The thickness of the emplaced sills was kept at 300 metres and the frequency of emplacements was kept the same with a period of 400 years between individual intrusions. This high emplacement rate allowed the system to maintain high temperatures capable of sustaining high melt volume fractions well beyond those predicted by Paulatto et al. (2012) from the SEA-CALIPSO data. Using 300 metre thick sills slowed their cooling rate, allowing rapid melt segregation and accumulation into high porosity waves, with fresh melt entering the system before the previously emplaced sills cooled below their solidus temperature.

Reducing the total emplacement thickness by a third, to 2 km over the 23 ka run time, still left the maximum melt fraction at the top of the system well above that estimated from the Montserrat velocity model. In addition, the volume of the velocity anomaly was reduced significantly in comparison to that obtained from the SEA-CALIPSO seismic data. The total depth over which partial melt is found at the Soufrière Hills Volcano has been hypothesised as extending to depths beyond 12 km (Paulatto et al., 2012; Annen et al., 2014). Whether this were in the form of the double reservoir volcanic system used in purely thermal modelling or a 'mush' column as described by Caricchi and Blundy (2015b), the evidence for the presence of melt at depth suggests that the method of intruding smaller volumes using melt segregation would not be capable of matching the observational data.

It was considered therefore that multiple parameters had to be adjusted to reduce the melt fraction that accumulated during segregation to effectively reduce the synthetic velocity anomaly. Sill thickness was reduced and the interval between sill emplacements was increased in order to subsequently reduce the emplacement rate of melt in the shallow crust. This had the effect of substantially increasing the incubation time beyond the 23 ka model run time used for the purely thermal modelling by Paulatto et al. (2012).

The interval time between repetitive sill emplacements used in the purely thermal model of Paulatto et al. (2012) was based on observed data at Montserrat from lava flows and tilt-meter measurements. Field data suggested an historic interval of 400 years between eruptions during periods of relatively high activity at the Soufrière Hills Volcano (Paulatto et al., 2012; Annen et al., 2014). While the occurrence of an eruption during static modelling can only be associated with either a second boiling, or fresh influxes of melt and an over pressurisation of the system, it has been shown by previous modelling using melt segregation that melt accumulation is possible at the top of a plutonic system without having to bring in a large volume of molten material (Solano, 2011; Solano et al., 2012, 2014). Smaller intruded volumes are capable of yielding mobile, eruptible melt volume fractions when melt segregation is accounted for in the system due to the voracity with which melt accumulates (Jackson et al., 2005; Solano et al., 2012).

Results in section 5.4.4 verify the hypothesis that it would be possible to produce, and sustain, high melt volume fractions at emplacement rates much lower than those used in previous purely thermal modelling. In particular, it is clear from the results in figure 5.21 that the thickness of emplaced sills need not be large for melt to eventually accumulate once the shallow crust has been incubated. Emplacement rates in one-dimension of only 10 mmpa were capable of sustaining melt over a long

period of time, even when the initial emplacements were tested at much shallower depths, in cooler surroundings, than were used in the static model.

While eruption frequency may give an indication as to the frequency with which fresh melt fluxes occur in volcanic systems it is important to note that the total life time of the volcano must equate to the total time over which the system has experienced melt influxes. Therefore, chemical evolution would have been occurring over the total life time of the volcanic plumbing system, producing heterogeneous layers of SiO_2 content in the shallow crust as evidenced by figure 5.15. The resultant layers would have varying liquidus temperatures and would therefore be more susceptible to melting during the influx of fresh, high temperature melt into the system. As a volcanic system evolves over time it would therefore be possible for small volumes of intruding melt to result in large-scale melting of a mush column residing beneath an active volcanic centre. This would produce large volumes of mobile, eruptible melt in the shallow crust through melt segregation, without relying on extremely thick repetitive intrusions such as those used in static modelling.

The results shown in figure 5.21 most closely match the recorded velocity anomaly at the Soufrière Hills Volcano as can be seen from the comparison between panels a and e. There is a clear difference in the geometry of the low velocity zone however between the match from the purely thermal model and that of the thermo-mechanical model (panels b and e respectively). The main difference is due to the high dependence of seismic velocity on melt fraction and the difference in the melt fraction distributions between the two models. While the static model is only capable of producing a large liquid vat of melt in the high temperature region of the model, as shown in figure 5.23, melt segregation in the thermo-mechanical model has decoupled the locations of highest melt fraction and highest temperature. Additionally, the difference in the shape and size of the velocity anomaly can partly be attributed to the approximation used in estimating the lateral extent of diffusion. The original thermo-mechanical modelling was carried out in 1D and then extended into 2D using the equations described in chapter 4. This has led to a potential underestimation of the lateral extent of the velocity anomaly. The magnitude of this underestimation is estimated in the Appendix. As a result it is possible that a smoother geothermal signature and velocity anomaly may be predicted in the shallow crust when using the thermo-mechanical model with the inputs described for figure 5.21. This is because the higher lateral diffusion would result in lower overall temperatures of the system and may reduce the presence of melt lenses on the time scales used.

Another important factor to note is the difference in the resolution of the models. While the SEA-CALIPSO seismic experiment was shown by Paulatto et al. (2012) to have a maximum resolution at

depths of 6 km of only 2×5 km the high resolution thermo-mechanical model produces a velocity profile with grid spacing of only 15×15 metres. This resolution is greatly reduced by the interpolation used to smooth the model for use by the tomo2D package but it still remains higher than that used by the static model in the SEA-CALIPSO seismic experiment in order to make sure that the final results were not affected by a reduction in resolution.

Due to the lower emplacement rate used by the thermo-mechanical model, the temperature profile is a lot smoother and lower on average across the region (figure 5.23). The melt fraction distribution produced over 615 ka of 100 metre thick intrusions is much narrower vertically and suggests that it is possible to produce a broad seismic velocity anomaly, such as that observed by the SEA-CALIPSO experiment, with very low melt fractions. This supports the idea of a crystal rich mush column beneath sub-volcanic centres which only forms a transient magma chamber with a high volume of mobile melt immediately prior to eruptions (Annen et al., 2014).

The total model run time used in the final scenario plotted in figures 5.21 and 5.23 of 615 ka is much larger than the suggested age of the Soufrière Hills Volcano. The first eruption has been determined to have occurred over 250 ka (Rea, 1974; Loughlin et al., 2010). However, it is important to note that the time frame over which volcanism has been occurring on the island of Montserrat is between 11 - 25 Ma (Harford et al., 2002). Emplacements would have begun to occur within the sub-volcanic system beneath the Soufrière Hills Volcano well before it would have first erupted due to the incubation period required in the shallow crust to form eruptible melt volumes. While we would have expected some mafic melt to have risen through the crust during this time it may not have reached the surface. In addition, the Centre Hills Volcano is estimated to have gone extinct over 500 ka, suggesting that the time frame used for the thermo-mechanical model fits well with the time frame of historical activity and emplacements beneath the active volcanic centres on Montserrat.

5.6 Conclusion

Due to the static nature of purely thermal modelling, the only way to produce eruptible melt volume fractions in the crust is to use high melt emplacement rates which form crystal poor reservoirs. As a result, the observed seismic velocity anomaly from the SEA-CALIPSO survey at the Soufrière Hills Volcano has been explained by Paulatto et al. (2012) using high emplacement rates that produce large liquid vats as predicted by Bowen (1915a,b). In contrast, thermo-mechanical modelling is capable of producing highly evolved high melt fractions in the shallow crust that can be maintained at lower

temperatures. Accumulation of crystal poor melt in sub-volcanic systems therefore occurs over much shorter time scales when melt segregation, matrix compaction, and reactive flow are accounted for at the emplacement rates employed by static models.

The results shown in section 5.4.4 show that it is possible to produce a synthetic seismic velocity anomaly similar to that observed in the field beneath the Soufrière Hills Volcano when melt segregation is accounted for. However, it is important to note that the problem is not well bounded and the solution is non-unique. It would be possible to use a large variety of combinations of intrusion rates and emplacement styles to produce a final estimated velocity anomaly matching the observed anomaly from synthetic melt fraction and temperature distributions. 1D results show that the dependence of bulk modulus and seismic velocity on melt fraction dominates the sub-volcanic systems over the corresponding calculated temperature dependence.

Using a low emplacement rate of only 10 mmpa by intruding 100 metre thick sills via under accretion leads to a deep negative velocity anomaly estimated from the thermo-mechanical model results that closely resembles the recorded anomaly beneath the Soufrière Hills Volcano when filtered using the *tomo2d* package which has a resolution of 300 x 300 metres as seen in figure 4.21. The results shown in this thesis are for a total model run time of 0.615 Ma, which is more than the age of the Soufrière Hills Volcano but much less than the total amount of time over which volcanism has been occurring on the island of Montserrat (over 11 Ma). A longer run time for a larger number of separate emplacement episodes, all with an initial emplacement depth of only 4 km below sea level, would have developed a large sub-volcanic mush column. As the Soufrière Hills Volcano has only been active for approximately 250 ka, future work would benefit from a seismic survey over both a very young and a much older active volcano in order to be able to make a comparison and investigate the vertical extent and evolution of sub-volcanic mush columns.

Due to the non-uniqueness of the solution to the problem of attempting to replicate an observed seismic velocity anomaly using numerical modelling it is not possible to determine a single set of modelling parameters that describe the current state of the internal dynamics of the volcanic plumbing system at Montserrat. It is important to note however that the addition of melt segregation in the thermo-mechanical modelling better reflects the full physical system as it incorporates melt evolution and the movement of mass through the system. The only way to further narrow the bounds of the model would be for future work to include further field measurements from outcrops on Montserrat and where possible to take drill cores to assess the geology of the volcanic plumbing system. It is therefore concluded that future seismic surveys both at Montserrat and other volcanic sites should

include full geological surveys. This would not only benefit the academic community in deepening our understanding of volcanic processes but would also further the ability of numerical modelling to assess the internal structure of shallow volcanic systems and therefore improve forecasts of volcanic activity.

Chapter 6

Travel Time Tomography and Full Waveform Inversion Comparison at Montserrat

6.1 Background

Seismic reflection and refraction data are sensitive to subsurface velocity and have long been used to provide information about sub-surface strata, for shallow and whole-crustal targets. In the case of deeper targets, the acquisition of seismic reflection and refraction data is relatively expensive compared to other geophysical techniques, but has the advantage of having a better resolution than potential field, resistivity, and electromagnetic induction methods which additionally may not be possible (Morgan and Rebolledo-Vieyra, 2013). The resolution of seismic refraction data, when only travel-times are inverted to obtain a velocity model is approximately equal to the Fresnel width, but can also be further limited by the acquisition geometry (Williamson, 1991). Using a regularized 3D tomographic inversion of first-arrival travel-time data, Zelt (1998) showed that, in areas of good ray coverage, the lateral resolution was approximately equal to half the shot or receiver spacing, whichever is the largest. Thus, quite densely-spaced 3D surface arrays are critical for maintaining the horizontal resolution of the method. The petroleum industry regularly uses dense arrays however, academic active seismic experiments are historically much less frequent due to the high costs involved (McQuillin et al., 1984).

There exist relatively few seismic data sets over active volcanic regions, simply because they hold little interest for petroleum prospectors (Staples et al., 1997). The difficulty involved in imaging below active volcanoes has also had an impact on the number of studies that have been conducted in the past. Geologically complex overburdens and highly crystalline structures in shallow sub-volcanic regions of the crust result in scattering of seismic rays, leading to poor resolution images which hold little useful information on the velocity structure of the target site (Ziolkowski et al., 2003; Mackenzie et al., 2005). The poor information obtained from seismic surveys from academic studies has historically been a limiting factor when weighed against the costs involved in setting up and conducting conventional travel time tomography seismic surveys (Mackenzie et al., 2005).

Ordinarily, the extensive scattering from crystalline igneous structures coupled with attenuation of high frequencies impedes the recovery of sub-surface velocity when using classic travel-time inversion to image the subsurface (White et al., 2003, 2005). Wide-angled seismic studies have been successful in improving travel-time inversions in regions where the crustal composition is dominated by large igneous formations (Fruehn et al., 2001; Fliedner and White, 2001; Spitzer et al., 2005; Chironi et al., 2006). The use of wide-angle configurations and dense acquisition geometries has led to significant improvements in seismic reflection images (Pratt et al., 1996). However, wide azimuth data alone is

not sufficient for producing detailed high-resolution images of the sub-surface below active volcanoes (White et al., 2005). While the long offsets allow for deeper penetration and improved resolution, the inherently crystalline nature of the igneous rocks and the presence of basaltic sills still inhibits the imaging technology (White et al., 2005; Chironi et al., 2006). Despite numerous improvements in travel-time tomography over the last two decades, when used alone, the method is inherently incapable of producing the detailed images required for accurate measurement of sub-volcanic melt distribution (Hansen et al., 1999; Christeson et al., 2008; Virieux and Operto, 2009; Mattioli et al., 2010; Foroozan et al., 2010).

Inverted results from the wide-angle SEA-CALIPSO experiment carried out at the Soufrière Hills Volcano in Montserrat illustrate the limitations imposed on resolution using traditional seismic methods (Paulatto et al., 2012). The experiment included a total of 4414 shots and 247 seismometers, and checkerboard tests show that the resolution of the p-wave velocity model was only $8 \times 8 \times 4$ km (in the x, y, and z directions respectively) at depths between 2 - 6 km (Paulatto et al., 2012). At depths shallower than 2 km the resolution suffered further due to the sub-parallel nature of seismic rays. Below 6 km the resolution decreased significantly due to a lack of rays reaching these depths, as most turning points were between 5 - 6 km (Paulatto et al., 2012; Annen et al., 2014).

Full-waveform inversion (FWI) is a highly advanced, computationally expensive data-fitting method that is able to recover high-fidelity velocity models to a much higher resolution than travel-time tomography (Virieux and Operto, 2009; Warner et al., 2013). The vertical resolving power of FWI is on the order of only half the propagated seismic wavelength, making it capable of imaging fine-scale structures, including thin melt lenses, in sub-volcanic systems (Virieux and Operto, 2009).

The velocity model produced using FWI essentially represents the velocity field where a misfit function, defined as the difference between recorded and modelled seismic data, is at a minimum throughout the computational domain (Menke, 1984). The recorded and modelled seismic data have a non-linear relationship and, hence, the technique uses multiple iterations of the inversion, making the assumption that, for small updates, the relationship is close to being linear (Virieux and Operto, 2009). A linearised local inversion is used to update the starting model for each iteration with the calculated velocity field from the previous iteration, thereby eventually converging on a final model (Morgan et al., 2013).

FWI was first described theoretically by Tarantola (1984). The iterative approach outlined by Tarantola (1984) was thought to be too computationally demanding, but improvements in computer hard-

ware and advancements in FWI algorithms have dramatically reduced the computation time, making it a commercially viable technique for geophysical exploration (Sirgue et al., 2010a; Vigh et al., 2013; Warner et al., 2013). FWI is able to account for the entire seismic wavefield through honouring all of the physics involved in calculating wave propagation through a medium (Operto et al., 2013; Prieux et al., 2013a,b). The resulting solution is therefore theoretically capable of recovering a subsurface model describing any property that affects the propagation of seismic energy and, most importantly, the recorded seismic wave-field (Virieux and Operto, 2009; Kapoor et al., 2013; Operto et al., 2013; Warner et al., 2013).

While it would be possible to develop alternative sub-crustal parameter models, such as density or s-wave elastic models, commercial use of 3D FWI in the petroleum exploration industry commonly uses an acoustic approximation to the wave equation in order to be computationally efficient and effective, and therefore only p-wave velocity is usually recovered (Virieux and Operto, 2009; Kapoor et al., 2013; Warner et al., 2013; Morgan et al., 2016). FWI generally uses long-offset, low-frequency datasets in order to achieve and maintain a high resolution final velocity model at depths required for petroleum reservoir modelling (Sirgue et al., 2010a; Vigh et al., 2011, 2013). Applications of FWI for the petroleum industry focus mainly on improving the seismic reflection images produced from pre-stack or reverse-time depth migrations (Plessix and Perkins, 2010; Ratcliffe et al., 2011; Warner et al., 2013).

Until recently, academic studies principally used 2D FWI to obtain velocity models in order to investigate and improve understanding of various scientific targets (Collier and Singh, 1997; Kamei et al., 2012; Morgan and Rebolledo-Vieyra, 2013; Brenders and Pratt, 2007). A principal issue is that academic data are typical much sparser than industry data. In a recent 3D application of FWI to a sparse OBS dataset across an ocean spreading centre finer-scale velocity structures were recovered at resolutions of up to 4 times better than obtained using travel-time tomography (Morgan et al., 2016). While the SEA-CALIPSO seismic survey used a number of ocean bottom seismometers at large offsets to image beneath the active centre at the Soufrière Hills Volcano, the final dataset cannot be used for a full-waveform inversion, since the shot and receiver spacings were not dense enough, and the frequencies used were not low enough for FWI to be carried out on the recorded seismic data.

One of the most significant drawbacks of FWI is that the initial starting model used in the inversion process must be quite close to the true model for FWI to be successful (Sirgue, 2006; Warner et al., 2013). Due to the nature of local optimisation problems, FWI is sensitive to the accuracy of the starting model, with potential for an incorrect match between observed and predicted data being

high. As a result, making an accurate starting model is one of the key challenges to be overcome when attempting a high-resolution, high-fidelity recovery (Sirgue, 2006; Morgan et al., 2013). The starting model for FWI must be able to generate synthetic data that lies within half a cycle of the observed data at the lowest frequency used in the inversion (Sirgue, 2006). If a less accurate starting model is used cycle-skipping may occur where the inversion settles on a local rather than global minimum of the objective function (Sirgue, 2006; Morgan et al., 2013). There are a number of techniques available for building starting models for a full waveform inversion including first-arrival travel-time tomography, stereotomography, and reflection tomography (Woodward et al., 2008; Virieux and Operto, 2009).

In the case of synthetic tests, building a sufficiently accurate starting model poses less of a problem than with observed seismic data because the true velocity model is known. Synthetic starting models can be developed simply by filtering the true synthetic datasets to remove fine-scale structure and give a realistic initial approximation, or they can be obtained using travel-time tomography (Virieux and Operto, 2009). The key objective in this chapter is to use synthetic tests to investigate the ability of FWI to recover subsurface velocity structure at a hypothetical multiple-sill intrusion site in order to explore how well FWI is able to recover the detailed structure across a relatively complex site of magma storage. Synthetic data are generated using a source wavelet and a p-wave velocity model for the volcanic intrusion zone, termed the true velocity model. FWI is then applied using these synthetic data as inputs and a simple, smooth starting model. The performance of FWI is then verified by comparing the true and recovered velocity models. In particular, a key issue which is investigated is the maximum frequency to which such a large dataset must be inverted to produce a high quality, high fidelity recovery of the velocity model.

6.2 Method

The 'true' velocity model was created from the temperature and melt fraction distribution predictions of the thermo-mechanical model shown in figure 5.23 of chapter 5. The starting parameters for the thermo-mechanical model are listed in table 6.1, and the resulting p-wave velocity model is shown in figure 5.21. Travel-time tomography was used to obtain a starting velocity model for FWI. The C++ 2D joint refraction and reflection travel-time tomography package developed by Korenaga et al. (2000) called 'tomo2d' was used to generate synthetic travel time data, and a 1D starting velocity model (figure 5.23) was used for the travel-time inversion. It is not possible to use very small grid

sizes in tomo2d, which meant that the true velocity model had to be resampled from a 15-m to a 300-m grid spacing, hence, the true velocity model for the travel-time tomographic inversion (6.1) did not contain fine-scale structure (anything >300 metres wide) across the sill intrusion zone and was, thus, much smoother than the 'true' model used for comparison in FWI. The 'true' model for FWI is shown in figure 6.3b alongside the starting model taken from tomo2d (6.3a) which has been converted from depth on the y-axis into travel-time in milliseconds.

For FWI, a 2D, isotropic, acoustic code developed by the Imperial College FWI Research Team was used in order to be computationally efficient. Although the Imperial fullwave code has the capability to analyse 3D datasets, be elastic, and include the effects of anisotropy and attenuation, all of these significantly increase the run time (Warner et al., 2013). For the synthetic tests shown here, the purpose is to investigate how well FWI can recover subsurface p-wave velocity structure across a sill intrusion zone, and there is no additional benefit in using the full physics. In addition, the synthetic test is designed using a dense shot and receiver spacing in order to ensure that the experimental geometry does not adversely affect the resolution. There are 274 shots, spaced 90 m apart, located at 15 m below the sea surface; and 137 receivers, spaced 180 m apart, located on the sea-bottom at 1005 m depth.

The grid spacing of the velocity model is 15 m across the domain which was 14 km wide in total, which means that the maximum inversion frequency is approximately 25 Hz (minimum velocity/ $(4 \times \text{grid size})$) (Davy et al., 2017). One of the constraining factors on resolution when running FWI is the maximum inversion frequency, since resolution is approximately half the seismic wavelength and this gets smaller with increasing inversion frequency. The FWI run-time scales with the number of cells in the model, with run time increasing by an order of magnitude when the grid resolution is halved. Hence, for large 3D model sizes such as expected for the case of sub-volcanic intrusion zone, high-frequency inversions up to the maximum inversion frequency may not be affordable. For this reason the results after inversions of 4 Hz, 6 Hz, 10 Hz and 17.5 Hz are shown in order to explore how maximum inversion frequency affects velocity recovery.

Symbol	Unit	Value
z	Sill thickness (m)	100
r	Emplacement rate (mmpa)	10
ϕ_0	Melt fraction	1
x_0	Initial emplacement depth (m)	400
dt_0	Time interval between emplacement (yrs)	10000
t_{final}	Total run time of simulation (yrs)	615000
t_{int}	Time interval between episodes (yrs)	15000
k	Thermal conductivity ($\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$)	3.0
L_f	Latent heat of fusion ($\text{Jk}^{-1}\text{K}^{-1}$)	550000
ω	Pluton width (m)	1000
z_{total}	Total emplaced thickness (m)	6000
T_L	Liquidus temperature (K)	1223.15
T_S	Solidus temperature (K)	973.15
ρ_s	Density of solid (kgm^{-3})	2500
ρ_m	Density of melt (kgm^{-3})	2000
ρ_w	Density of sea water (kgm^{-3})	1000
v_w	Seismic velocity in sea water (ms^{-1})	1500
K_m	Bulk modulus melt (GPa)	12.7
μ_m	Shear modulus melt (GPa)	0

Table 6.1: Parameters used in the segregating case of the thermo-mechanical model to compare against the static results of Paulatto et al. (2012). The simulation used two emplacement episodes separated by a time interval, t_{int} . Sills were emplaced via under accretion.

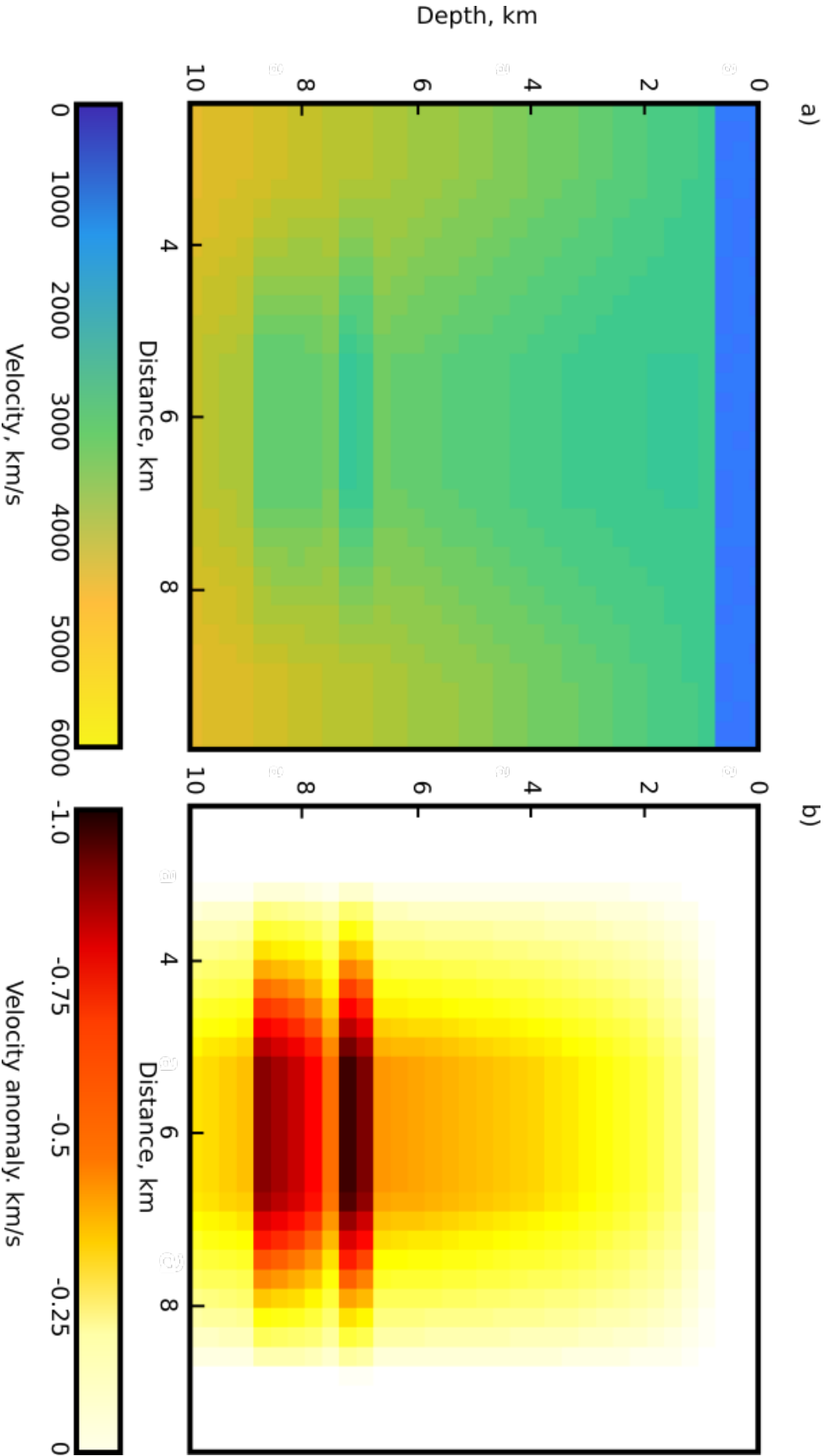


Figure 6.1: a) The 2D velocity profile resulting from an inversion of the smoothed estimated velocity model using the `tomod2d` travel time tomography package. b) The corresponding velocity anomaly when the inverted velocity field is subtracted from the background velocity gradient.

6.3 Results

Figure 6.2 shows a comparison between the starting (a), recovered (b), and true (c) velocity models for tomo2d from the thermo-mechanical model shown in figure 5.21. The starting model used was simply the background velocity gradient from the thermo-mechanical model with no velocity structure in the sub-volcanic zone as can be seen in panel a. The true model was a smoothed version of the final results of the conversion of the thermo-mechanical modelling results into seismic velocities using the methods outlined in chapters 3 and 4. Grid spacing for the true model was reduced from 15 metres to only 300 metres so as to be more in keeping with the resolution observed in Paulatto et al. (2012). The difference between the starting and recovered model is very clear, with a low velocity zone recovered between 6 - 8 km depth. However, the recovery can be seen to be of a much smaller magnitude than the 'true' model shown in figure 6.2c. In particular, it can be seen that the deeper low velocity anomaly in the true model between 7.2 - 8 km depth has not been well recovered. The horizontal extent of the recovered anomaly is also smaller than the true anomaly using the synthetic travel-time tomography inversion software package. The recovered model shown in panel b was subsequently used as a starting model for FWI.

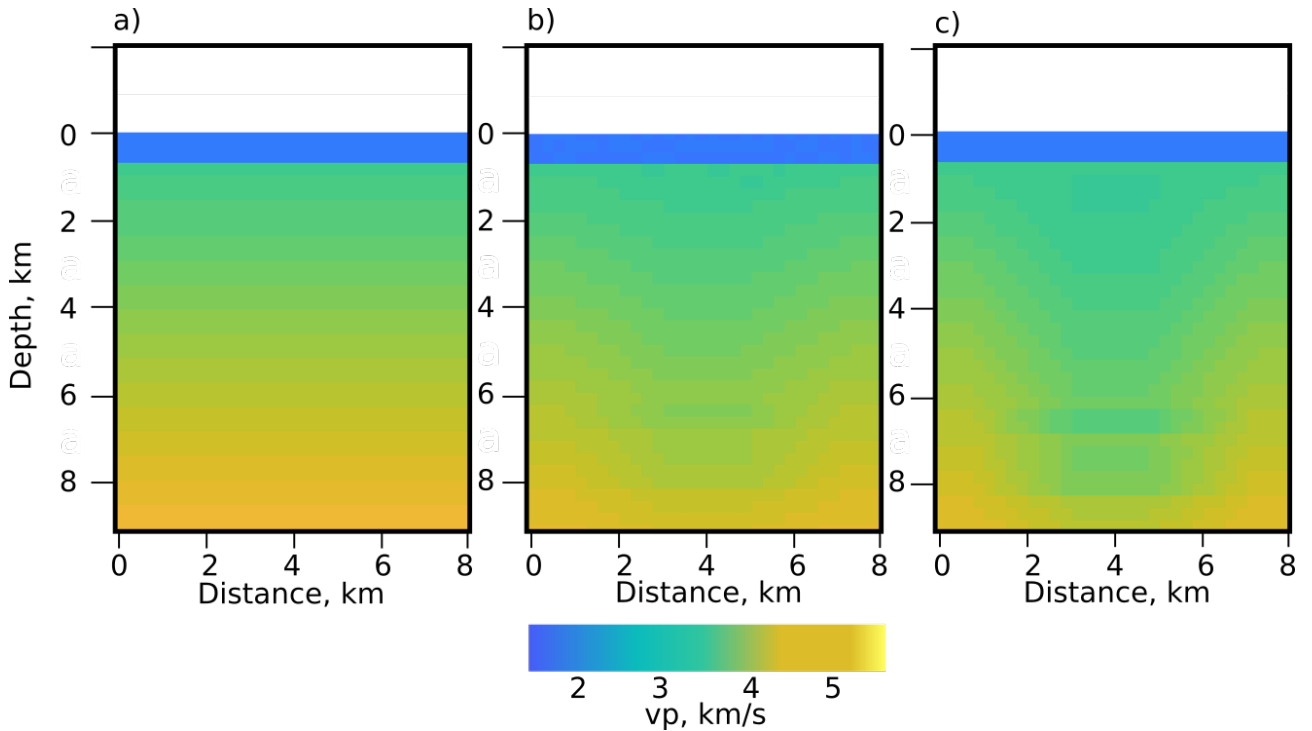


Figure 6.2: Starting (a), recovered (b), and true (c) models for the synthetic travel-time tomography inversion carried out using the software package tomo2d on the results from the thermo-mechanical model shown in figure 5.21.

Figure 6.3 shows a comparison between the starting model used for the FWI (6.3a), recovered using the tomo2d package, and the 'true' velocity model used for comparison in the FWI, which was produced from the thermo-mechanical model using the methods outlined in chapters 3 and 4. The wider grid spacing used in the travel-time inversion (300 metre wide grid spacing) has resulted in much of the fine-scale velocity structure, which can be seen in the high-resolution true model (15 metre wide grid spacing), not being recovered. The final recovered velocity model using FWI can be seen in figure 6.4 which shows a comparison between the central section of the recovered velocity model domain (between CDP 580 and 1120) from both tomo2d (6.4a) and FWI (6.4b). This section contains the velocity anomaly produced by the modelled pluton emplacement zone. The FWI was run using a maximum frequency of 17.5 Hz in 2D. While both models show a similar background structure, with a low velocity zone between 7000 - 9000 ms, the recovery using FWI clearly contains a number of narrow low velocity layers, with p-wave velocities as low as 3.09 km s^{-1} that can be seen between 7000 - 8000 ms and were too small to be recovered using the tomo2d travel-time inversion package. The resolution in the recovered velocity model using FWI can be seen in figure 6.4 to be approximately 4 times better than that obtained using the tomo2d travel-time tomography package.

Figure 6.5 shows a comparison between the final recovered velocity anomalies using FWI at frequencies of a) 4 Hz, b) 6 Hz, c) 10 Hz, and d) 17.5 Hz. The true velocity anomaly is shown in panel e) along with the true velocity model in panel f). The recovered velocity anomalies were calculated by subtracting the final result from the inversions at increasing frequencies from the initial starting model to determine the extent to which the fine-scale velocity structure could be recovered at the various frequencies used.

Panel a) can be seen to contain less structure, with only three very thin velocity anomalies recovered at 7900 ms, 9000 ms, and 9500 ms. This inversion was run only to 4 Hz and the anomaly here can be seen to be much narrower, only approximately 100 CDPs or 500 metres wide, than the 'true' anomaly shown in 6.5e and has not been able to recover the shallow melt lenses seen in the 'true' anomaly immediately below 7000 ms. While this result shows that higher frequencies are required to produce meaningful final velocity anomalies, it is helpful in that it shows that the velocity perturbations recovered up to this point are of the correct sign and in the correct approximate location. The absolute size of the recovered anomaly improves immediately when the inversion is run up to 6 Hz as shown in 6.5b. The fine-scale structure is immediately more apparent, with the locations of three thin melt lenses recovered between 7000 ms and 7500 ms. The anomalies again have the correct sign and location however they are thinner than those seen in the true model and the structure between 7500 - 8000 ms has not been recovered. In addition, the absolute value of the anomaly seen in panel b) is

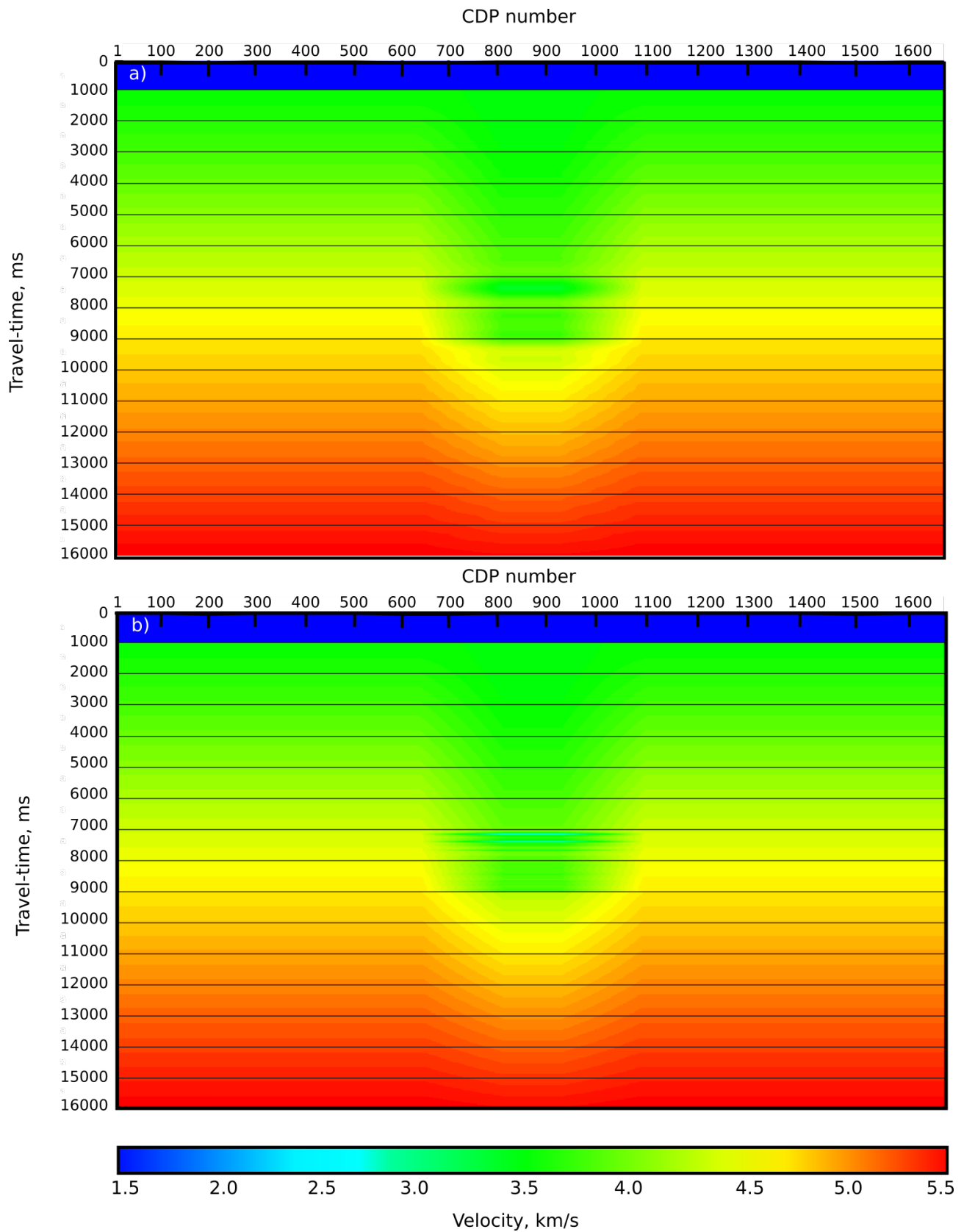


Figure 6.3: Starting (a) and true (b) models for the FWI. The starting model has been converted into milliseconds from depth results of the tomo2d inversion.

smaller than that of the true model, with the recovered positive anomaly at 7100 ms reaching only 200 ms^{-1} . This is most apparent in the deeper negative anomaly at 9000 ms which can be seen to be much smaller in absolute value (only -100 ms^{-1}) than that in the true model (-250 ms^{-1}).

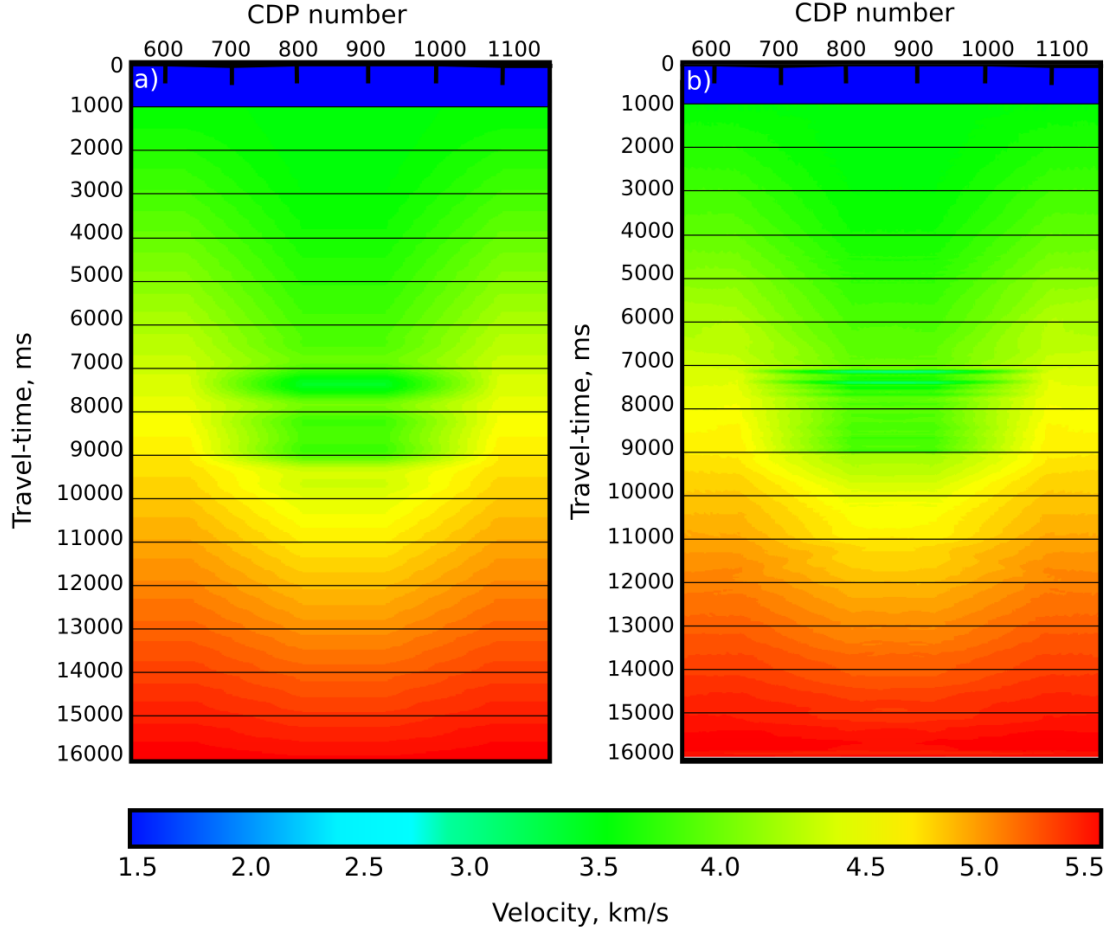


Figure 6.4: Comparison between the recovered velocity models from a) tomo2d and b) FWI after being run up to 17.5 Hz.

Further improvements to the size of the recovered velocity anomaly can be seen once the inversion has reached 10 Hz (6.5c). The width of the anomaly shown in panel c) is approximately 350 CDPs wide, corresponding to over 1.5 km. The absolute values of the alternating negative and positive anomalies recorded between 7000 ms and 7500 ms are also closer to those in the true model, reaching up to $\pm 200 \text{ ms}^{-1}$. It is clear however that the anomaly at 7900 ms is too large in comparison to that in the true model and there is a lack of fine-scale structure at 10 Hz observed between 7500 ms and 8000 ms.

Following this, the inversion was then run using a much higher frequency of 17.5 Hz, shown in 6.5d. The recovered velocity model in panel d) shows the great improvements provided by increasing the maximum inversion frequency. The top-most negative velocity anomaly matches well in location, size, and absolute value with that seen in the 'true' model. In addition, the upper-most positive anomaly recorded at 7100 ms can be seen to be very similar to that in the 'true' model, with a width between CDP numbers 680 - 1020. Below this, the recovered anomaly reduces in width in 6.5d in comparison to the true model, with the positive anomaly recorded at 7500 ms being only approximately 200 CDPs wide as opposed to 350 CDPs wide in the true model. The absolute values of the anomalies at these depths however match very closely with the true model at $\pm 230 \text{ ms}^{-1}$. The fine-scale velocity structure between 7600 - 7800 ms is underestimated in the recovery at 17.5 Hz, with the negative velocity anomaly at 7600 ms being only partially recovered both in terms of its width and the size of the anomaly, which can be seen in panel d) to be only -50 ms^{-1} in comparison with the true anomaly of -230 ms^{-1} . Conversely, the positive anomaly recorded in panel d) at 7900 ms has been overestimated and can be seen to be larger than that in the true model. The deeper anomaly recorded at 9000 ms is smaller than that seen in the true model, being only 250 CDPs wide, and 100 ms thick however the absolute value of the centre of the anomaly matches well with the true model in 6.5e.

A narrow positive anomaly can be seen at approximately 9500 ms in all of the velocity anomalies recovered using FWI which does not exist in the true model. This occurs at the location of the steep velocity contrast at this depth seen in 6.5f at the base of the emplacement zone.

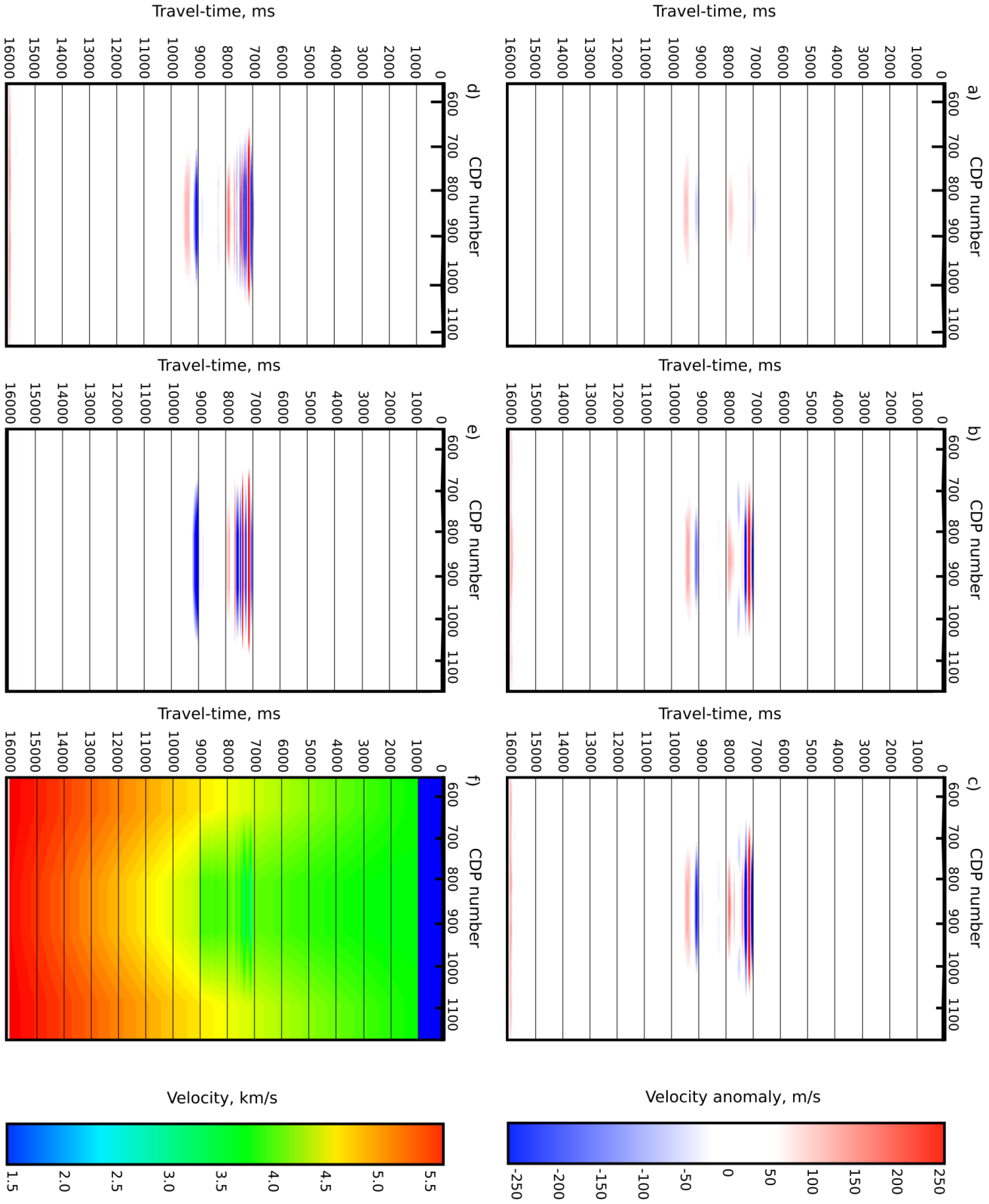


Figure 6.5: a)-d) Recovered velocity anomalies from FWI run to 4, 6, 10, and 17.5 Hz respectively. e) True velocity anomaly used in FWI. f) True velocity model for FWI.

6.4 Discussion

Figure 6.4 displays a significant improvement between the recovered velocity models using FWI over the travel-time tomography package developed by Korenaga et al. (2000), *tomo2d*. Recovery using FWI can be seen to be up to ten times better than that using *tomo2d*, with the three thin melt lenses observed in figures 5.21 and 5.23 clearly visible in 6.4b. The high melt fraction lenses can be seen in 5.23 to be less than 100 metres wide and as such were not able to be recovered using travel-time inversion, which has a resolution of approximately 1000 metres at these depths and velocities. At the highest frequency used in the FWI, 17.5 Hz, the resolution at these depths and velocities is approximately 120 metres although it is important to note that it is possible for smaller structures such as the melt lenses to be detected but their widths may not be accurately recovered. Evidence for the recovery of most of the fine-scale structure in the inversion run using FWI suggests that the dense shot-receiver spacing used in the synthetic inversion could be applied in real case studies to achieve high-fidelity, high-resolution recovery of sub-volcanic velocity structures if the model predictions are correct. It is also important to note that testing at various frequencies showed that the inversion run using FWI does not suffer from effects such as cycle-skipping. This is mainly due to the accuracy of the model recovered by *tomo2d* used in the inversion and shows that the travel-time inversion is capable of producing well recovered FWI starting velocity models despite its low resolution.

The results shown in figure 6.5 examine the potential improvement in the recovered velocity model provided by inverting to high frequencies. It is clear that the recovered models that were run only to low frequencies (6.5b and c) lack the fine-scale velocity structure recovered in figure 6.5e and are less close to true model. FWI is not able to recover the full scale or size of the anomalies created by the high melt fraction lenses at these frequencies despite the 15 metre grid block size and the dense shot and receiver spacing used. However, inverting at 10 Hz and at 17.5 Hz shows a significant improvement in the match between the recovered velocity model and the true model shown in 6.5. The amplitude of the anomaly is well recovered at depth and the scale of the anomaly matches the true model well. Much of the fine-scale velocity structure included in the true model can be observed to have been resolved at 17.5 Hz in the centre of the emplacement zone.

Total run time of the FWI carried out to 17.5 Hz to produce the final recovered velocity models shown in figures 6.4 and 6.5 was approximately 6 hours on Imperial College's CX1 computer, for a 2D inversion on a grid spacing of 15 metres over a model domain size of 20×16 km. The 2D inversions used a maximum inversion frequency of 17.5 Hz over 150 iterations. The 3D inversions shown in

Morgan et al. (2016), which had a model size of 27x20x6 km, a 50 metre grid spacing, and 21 Ocean Bottom Seismometers (OBSs). This used a similar computational resource in terms of the allocated nodes and CPUs on the CX1 cluster as the 2D FWI inversions shown in figure 6.5 to invert up to a maximum frequency of 5 Hz over 50 iterations. Despite having a much lower maximum inversion frequency, using fewer iterations, and having a wider grid spacing, the 3D model shown in Morgan et al. (2016) took approximately 24 hours to run due to the increase in model parameters attributable to running in 3D.

While the results in 2D at 17.5 Hz show the best match with the true velocity model it is apparent from the time taken for the 3D model to run that it would be computationally expensive to perform FWI on a large-scale dataset beneath an active volcanic centre. As maximum inversion frequency is increased, the node spacing and sample times must be reduced for the FWI. Consequently, doubling the maximum inversion frequency increases the run time by a factor of 2^4 , or 16 times in 3D. Thus for the model shown in Morgan et al. (2016), doubling the maximum inversion frequency used from 5 Hz to 10 Hz would result in a total run time of the FWI of approximately 16 days if the same computational resources were used. If this were applied to a FWI of a sub-volcanic system, the total model domain dimensions would need to be substantially increased in order for the full plumbing system to be imaged at depth. In addition, the number of sources and receivers used would have to be increased to achieve a dense enough array such that the resolution of the recovered velocity model would not be adversely affected. Once all of these considerations are taken into account the total model run time would be on the order of $10 - 10^2$ days to run FWI only up to 10 Hz, depending on the computational resources allocated to the inversion. As a result, it would be computationally expensive to achieve the resolution shown in figure 6.5 when inverting a real dataset beneath an active volcano.

Furthermore, the signal-to-noise ratio at active volcanic centres for seismic experiments is generally quite high due to the complex crustal geometry (Paulatto et al., 2012). This proved to be a serious problem for the SEA-CALIPSO experiment where it was found that the long history of volcanic activity made it incredibly difficult to detect a consistent reflection for the acoustic basement in the region (Paulatto et al., 2010, 2012). The issues related to signal-to-noise ratio would be expected to be prevalent at all volcanic centres however the use of simple windowing on early arrivals in FWI would dramatically improve the signal-to-noise ratio (Morgan et al., 2013). In addition, it would be possible to improve the signal at lower frequencies for FWI by towing the airguns for the marine acquisition at greater depth (Morgan et al., 2013).

6.5 Conclusion

Using the velocity model recovered from the travel-time tomography package, *tomo2d*, as a starting model for FWI resulted in a final inversion which showed no evidence of issues such as cycle-skipping. The final 2D inversion showed a good match in the resulting velocity anomaly recovered from the synthetic data of a sub-volcanic plumbing system. The fine-scale structure of the thin melt lenses predicted by the thermo-mechanical modelling was well recovered when the FWI was run up to high frequencies (above 10 Hz).

The lateral extent of the seismic velocity anomaly predicted by the thermo-mechanical model has been underestimated due to the 1D nature of the modelling process. The magnitude of this underestimation is estimated in the Appendix. It has been determined that the effect of this on the recovery of the fine-scale velocity structure using FWI is negligible due to the nature of seismic imaging. Steep velocity gradients may cause issues with seismic imaging (although the effect is greater for reflection tomography than for refraction tomography which is used for the synthetic imaging carried out in this thesis), and therefore the underestimation of the lateral diffusion results in a more complex recovery process using FWI. Seismic energy generally struggles when it comes to penetrating basalts, which causes challenges for travel time tomography and large lateral velocity variations can introduce non-normal moveout that further distorts imaging (Planke et al., 1999; Chironi et al., 2006). However, when imaging sharp lateral gradients, it has been shown that FWI is far more capable at resolving high-fidelity images than travel time tomography, this is supported by the good recovery of the individual melt lenses using FWI (Warner et al., 2013; Morgan et al., 2016; Martin et al., 2017).

Low seismic frequencies are required in order to image long wavelength features such as the individual melt lenses predicted by the thermo-mechanical model. The synthetic tests started at 3.4 Hz and were therefore able to recover both lateral and vertical velocity gradients very well. Sharp contrasts are often simply not picked up by travel time tomography, as can be seen from the synthetic modelling using *tomo2d* as well as in Paulatto et al. (2012). Sharp contrasts may also cause problems in FWI starting models, and Warner et al. (2013) have shown that they ought to be smoothed in starting models in order to avoid the inversion from converging on a local minimum during early iterations of the FWI. In effect this is already handled by using the synthetic travel time tomography *tomo2d* results in this thesis because the starting model for FWI is already smooth and also comparatively accurate. This means that the location of the sharp boundary is already well represented and so when

starting at low frequencies it is possible to have good recovery of the velocity structure despite the high true velocity gradients.

Warner et al. (2013) showed that if the contrast is less than half a wavelength at the lowest frequency then recovery should be possible. So, for the case of the final modelling carried out in this thesis, starting the inversion at 3.4Hz coupled with the shallow depths at which there are steep contrasts (where the sills are emplaced, 4 km), the background velocity can be estimated to have been 4.3 km/s, so respectively half the wavelength can be calculated to have been 720m (2sf). In the modelling used in this thesis, the lateral distance for heat diffusion is on this scale so the velocity gradient can be shown to be able to be well recovered. In addition, in the final model inverted using FWI, the lateral distance over which we see a velocity anomaly is much greater than this (on the order of kms) as the model ran for a longer time with smaller sill intrusions and so the sharpness of the lateral velocity gradient presented no challenge to FWI which was able to recover the low frequency, long wavelength information from the starting model in the first stages of the iterations. Underestimation of the lateral extent of the anomaly therefore poses no problem to FWI in this thesis. A greater diffusion distance across the horizontal extent of the model may in fact improve recovery due to shallower velocity gradients.

There is a clear trade off between the improvements to the recovered velocity model using FWI resulting from inverting up to high frequencies, and the computational expense involved. Doubling the maximum inversion frequency for a 3D inversion results in an increase in computation time on the order of 2^4 . As a result, it is concluded that the additional computational time makes it challenging to invert to high frequencies on real, 3D datasets across an active volcano. The improvement seen between recovered velocity models in 2D at 10 Hz and 17.5 Hz suggest that the recovery is sufficient at 10 Hz to provide a good understanding of the fine-scale velocity structure at active volcanic centres. The majority of the internal structure within the emplacement zone could be seen to have been well recovered at 10 Hz and the size of the anomaly was a good fit with the true model.

Chapter 7

Conclusion and Future Work

7.1 Summary and conclusions

The main hypothesis underlying the work presented in this thesis was that the geometry and evolution of magma storage systems beneath active volcanoes could be modelled using a thermo-mechanical model using substantially lower melt emplacement rates than has historically been used in purely thermal, static modelling. Further, it was hypothesised that the predicted temperature and melt fraction distributions determined by the thermo-mechanical model could be converted into an estimated seismic velocity field and compared to velocity models obtained from seismic refraction data.

With these aims, the results of the purely thermal model were benchmarked against those of the thermo-mechanical model when the melt segregation and matrix compaction terms in the system of governing equations were turned off. This was done to show that the thermo-mechanical model was capable of reproducing the results of the purely thermal model in a static scenario. Once the thermo-mechanical model had been shown to have satisfied a number of benchmarking tests it was used to reproduce the inverted temperature and melt fraction profiles calculated by Paulatto et al. (2012) for the shallow crust beneath the Soufrière Hills Volcano in Montserrat. Repetitive intrusions of sills into the shallow crust were simulated at a variety of emplacement rates and over a number of time scales to determine the best match of resulting temperature and melt fractions with velocity models obtained using the SEA-CALIPSO seismic data.

Temperature and corresponding melt fraction distributions in the shallow crust predicted from simulations that included melt segregation, reactive flow, and matrix compaction were then converted into estimations of bulk and shear moduli. The conversion was carried out using a combined approach of Karato's method for the effect of temperature on seismic velocity and Berryman's self-consistent method for calculating the effect of melt fraction on seismic velocity. Tests were run on the estimated values for bulk and shear moduli to ensure that they lay within the Hashin-Shtrikman bounds. Benchmarking against previous work provided a clear indication that the method used in this thesis was valid for the systems under consideration. While small discrepancies existed between the results obtained in this thesis and those derived from previous work it was determined that these could be accounted for by the use of different input parameters in the modelling.

Following determination of the elastic moduli at each point in the modelled sub-volcanic system, a corresponding estimation of p-wave velocity was carried out. A 2D velocity profile was then interpolated from the 1D results using the method as laid out in the Appendix for lateral diffusion of heat

from the edge of the pluton. The final 2D velocity profile was then compared against the velocity models obtained from the SEA-CALIPSO seismic experiment. In addition, it was compared with the velocity models derived from temperature and melt fraction distribution estimations at the Soufrière Hills Volcano calculated by Paulatto et al. (2012) using a purely thermal model.

The final results of the thermo-mechanical modelling carried out in this thesis show that the predicted spatial and temporal evolution of melt fraction distribution in shallow-crustal sub-volcanic systems is significantly different from that found in previous static modelling. When melt segregation coupled with matrix compaction is taken into account in the system of governing equations it is possible to accumulate high volume, eruptible mobile magmas at much lower emplacement rates than those used in purely thermal modelling. The results also suggest that with melt segregation, emplacement rates >750 mmpa used in Paulatto et al. (2012) and in various results shown in Annen et al. (2014), would result in the formation of unsustainably vast liquid reservoirs. Large quantities of crystal poor melt in the crust are buoyant relative to the surrounding solid country rock and would produce an over-pressurised system that would be likely to erupt (Petford and Koenders, 1998; Annen and Sparks, 2002). They are therefore unlikely to be sustained in a shallow sub-volcanic system. Rather, they are transient features that signify an imminent eruption. As a result, if the thermo-mechanical model is correct, the average rate at which melt intrudes so that highly crystalline, low melt fraction lenses reside in the shallow crust must be low to reproduce the velocity signature seen at Montserrat.

The necessary changes to the input parameters when segregation was accounted for included using an emplacement rate of only 10 mmpa (in contrast with 750 mmpa for the static model), with repetitive emplacement of sills only 100 metres thick. These low emplacement rates were required in order to avoid producing a large, liquid filled magma chamber which does not match field or geophysical observations for Montserrat. This resulted in a longer incubation period in the shallow crust and a total model run time of 615 ka. However, this time frame was shown to fit well with the time scale over which the island of Montserrat, and the Soufrière Hills Volcano, have been active (Rea, 1974; Loughlin et al., 2010). Results from the conversion of temperature and melt fraction profiles into seismic velocities using the methods outlined in chapters 3 and 4 show that the dependence of velocity on melt fraction is greater than that of velocity on temperature. Locations of high melt fraction lenses dominated the calculated velocity anomalies. This was particularly evident in the thermo-mechanical model where the location of highest melt fraction was decoupled from the location of highest temperature and the effect of melt fraction on the bulk modulus and velocity profiles could be clearly distinguished from that of temperature.

Reducing the emplacement rate of melt in the shallow crust resulted in a final velocity profile similar to that obtained by travel-time tomographic inversion of the SEA-CALIPSO data, with a broad average velocity anomaly of -0.51 km s^{-1} . However, the fine-scale structure present in the high resolution velocity profile estimated from the thermo-mechanical model results included thin high melt fraction lenses with a maximum negative velocity anomaly of -1.81 km s^{-1} are too small to be detected with travel-time tomography. When a filter was applied to generate a velocity model of appropriate resolution, a maximum negative velocity anomaly of -0.61 km s^{-1} was observed which matches more closely with the observed velocity anomaly beneath the Soufrière Hills Volcano. Most significantly, it is concluded from the thermo-mechanical modelling that the average 1D rate at which melt is emplaced into the shallow crust can be dramatically lower (on the order of 10^2 mpa lower) than has historically been predicted by static modelling to still produce large low velocity zones beneath volcanic centres.

Finally, an inversion was carried out using the recovered velocity profile from the synthetic travel-time tomography as a starting model for FWI. The aim was to determine whether substantial improvements in the recovered seismic velocity profile could be obtained from inverting the full seismic wavefield. The maximum inversion frequency is one of the key limiting factors when running FWI since the final resolution is approximately equal to half the seismic wavelength, which is inversely correlated with increasing inversion frequency. FWI run time scales with model size, increasing by an order of magnitude when the grid resolution used is reduced by half. Subsequently, large datasets such as those expected for 3D inversions of sub-volcanic plumbing systems would be computationally extremely expensive. Inversions at various increasing frequencies were compared to explore how the maximum inversion frequency affects velocity recovery and thus the viability of running a large-scale, 3D FWI on a sub-volcanic target. The results were also used to determine the extent to which FWI could improve the resolution of the recovered anomaly in comparison with travel-time tomography and therefore improve our understanding of the target site. FWI was performed on the synthetic velocity profile estimated from the thermo-mechanical model using the smooth profile recovered from tomo2d as the starting model.

It was found that the recovery using FWI was much improved in comparison to the travel-time tomography results, with a great deal of the fine-scale velocity structure seen in the final image despite the high velocity contrasts at the edges of the magmatic system. The recovered model using travel-time tomography showed only a broad low velocity zone at the depth of the emplaced pluton whereas FWI was able to recover the position of multiple thin, individual high melt fraction lenses. It was therefore concluded that FWI would be able to provide a much greater understanding of sub-volcanic structure and could be used in future academic studies at active volcanic centres to improve imaging

of the spatial distribution of melt in volcanic plumbing systems. Underestimation of the lateral extent of the seismic velocity anomaly was determined not to have impacted the ability of FWI to recover the fine-scale detail of the velocity structure due to the use of an accurate starting model produced using tomo2d and low initial inversion frequencies.

Comparing the inversion using travel-time tomography with that using FWI on the synthetic data shows that the final velocity anomaly using FWI has approximately ten times the resolution of the traditional travel-time inversion. While the resolution of FWI may be reduced on real data sets if they use comparatively sparse shot and receiver spacings, the improvement suggests that it would be possible to obtain very high resolution images using FWI if dense acquisition geometries are used in academic surveys. In addition, the results show that building starting models from travel-time tomography produces a good initial fit for the iterative approach used in FWI, avoiding common issues such as cycle-skipping and the introduction of noise in to the data.

A comparison between the synthetic 'true' model and results of inversions run using FWI up to frequencies of 4 Hz, 6 Hz, 10 Hz, and 17.5 Hz was then made to examine the effect of maximum inversion frequency on velocity recovery. It is clear from the results that the inversion at 4 Hz was not able to recover the predicted shallow fine-scale velocity structure. The width of the positive anomaly at 7900 ms was underestimated to be less than 100 common depth points wide (approximately 500 metres). Increasing the final inversion frequency to 6 Hz and subsequently to 10 Hz immediately improved the recovery, with three narrow anomalies seen between 7000 - 8500 ms. The width of the recovered shallow anomaly improved to be more realistic in comparison to the true velocity anomaly however, the deeper negative anomaly at 9000 ms was seen to still be much smaller than in the true model. The maximum inversion frequency used was 17.5 Hz which showed a very good recovery of the fine-scale structure. Increasing the inversion frequency produced a final anomaly whose size and depth matched closely to the true model and was determined to be a very good fit. The final inversion took approximately 6 hours to run at 17.5 Hz in 2D with a grid spacing of 15 metres. While the maximum inversion frequency for a 15 metre grid size was calculated as being approximately 25 Hz it was determined that this would be challenging to run inversions up to these frequencies using 3D FWI on a real sub-volcanic target with model sizes of a few 10s to 100s of kilometres.

7.2 Future work

The results shown in this thesis were carried out on synthetic velocity profiles developed using the methods outlined in chapters 3 and 4. In order to investigate the true resolving capabilities of FWI on academic datasets in the sub-volcanic crust it is necessary for a long-offset seismic survey to be carried out at an active volcanic centre using a dense acquisition geometry. The results using a recorded dataset would provide a detailed understanding of the true recovery resolution of FWI.

Implementing FWI on datasets from a number of active volcanic centres with varying ages would also give insight into the spatio-temporal evolution of melt fraction distribution in volcanic plumbing systems. It is hypothesised that a comparison between volcanic systems of different ages and at different stages in volcanic cycles would give a better understanding not only of average melt emplacement rates but also of the time scale over which melt is sustained in the shallow crust immediately prior to an eruption.

Broad negative velocity anomalies that have been shown using travel-time tomography to extend to large depths in the crust may denote the presence of mush column, as predicted by previous models of melt segregation. Carrying out FWI at active volcanic centres in future studies would improve imaging of these mush columns and enable scientific researchers to determine their vertical extent. An advantage of FWI over travel-time tomography is that its resolution capacity is as small as half the propagated wavelength, as opposed to only half a Fresnel width. As a result, it would theoretically be possible to image the mid crust to a high enough resolution using FWI to determine the fine-scale velocity structure of the mid-crust. Detailed images of the mid-crust would give a much improved understanding of the feeding system for volcanic plumbing systems. In addition, it would provide evidence to determine the validity of the hypothesis for highly crystalline mush columns existing below volcanic centres. Future work could use the methods outline in this thesis to estimate the melt fraction distributions, emplacement rate, and emplacement style of melt required in the mid-crust to produce the observed velocity structure to depths well beyond those previously imaged using travel-time tomography.

The thermo-mechanical model used in this thesis extends only in 1D whereas recent purely thermal models such as that developed by Annen (2009) use a 2D half-width domain with a mirrored edge through the centre of the modelled section to provide a full 2D profile. The extrapolation into 2D that has been used in this thesis was deemed sufficient and valid for the purposes of this work due

to the estimations involved in the calculations. However, converting the full system of equations into 2D would provide a much more in depth understanding of the dynamics in sub-volcanic systems. A further extension into 3D would further improve the modelling by including lateral movement of heat and mass. This would provide a more detailed physical estimation of the spatio-temporal evolution of melt distribution in the system and improve the mechanics of the modelling process.

On-going work is being under-taken to convert the thermo-mechanical model into a pseudo-3D system with cylindrical symmetry and it can be seen in figure 7.1a that the 2D thermo-mechanical model is able to closely reproduce the temperature results of static modelling by Annen (2009) when extended into 2D. However, further tests need to be carried out on the 2D model as there are differences in the melting relationships used in the thermal and thermo-mechanical models. These differences result in observable variations in the final results as evidenced by the lower melt fractions seen in 7.1b. Future work could use a final pseudo-3D version of the thermo-mechanical model to develop the elastic moduli and velocity conversion code into further dimensions. In addition, it would be useful to carry out a test to determine the bounds for the validity of both the thermo-mechanical and purely thermal models. While it is clear from current modelling as well as from testing by Solano et al. (2012, 2014) that the thermo-mechanical model incorporates additional complexities and so is helpful in providing an improved insight into sub-volcanic processes, it is important to determine the bounds of the model by running monte-carlo simulations to check the consistency of results under varying conditions and geometries. While this was not within the scope of this current work, it would be useful for future work to gain an improved understanding of the limitations of the themomechanical model.

Further on-going work is currently investigating joint inversions using gravity data alongside seismic inversions at active volcanic centres. Gravity data has been collected both onshore and offshore at the island of Montserrat. It would therefore be possible to conduct further seismic surveys to enable implementation of FWI at the Soufrière Hills Volcano and use the results alongside a gravity inversion to better constrain the structure of the lithology in the sub-volcanic crust (Moorkamp et al., 2011). Observed measurements from Kiddle et al. (2010) on crustal xenoliths from Montserrat could be used to determine the relationship between velocity and density in the region. In addition, the general empirical relationship described by Brocher (2005) could be used to provide estimated gravity anomalies from the results of melt fraction distribution from the thermo-mechanical model. This would enable gravity data to be jointly inverted with the seismic data and provide a more in depth understanding of the spatio-temporal evolution of melt in the volcanic plumbing system.

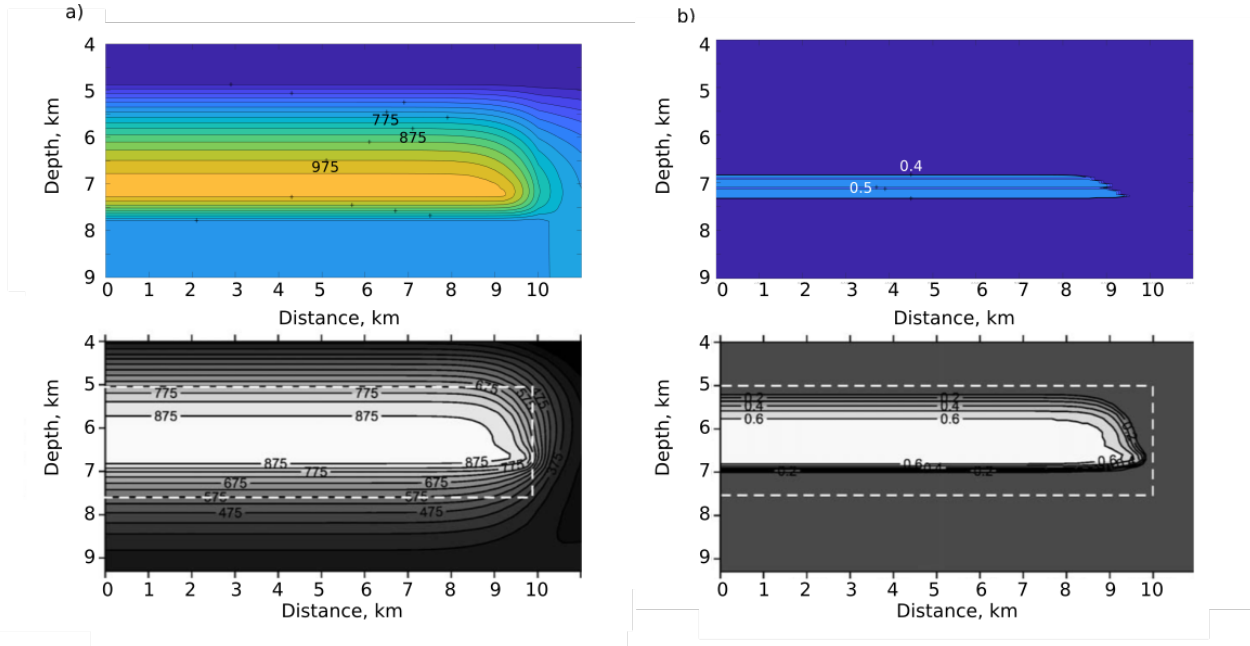


Figure 7.1: Comparison between a) the temperature results and b) the melt fraction results of the thermo-mechanical model (top) and the purely thermal model of Annen (2009) (bottom, taken from Annen (2009)) in 2D showing a good match in the static results.

Interferometric synthetic-aperture radar (InSAR) has been used to monitor surface displacements associated with active volcanoes, including taking measurements of dome growth at the Soufrière Hills Volcano in Montserrat (Wadge et al., 1999). It is suggested that future work include not only joint gravity inversions but also data collected using InSAR. Measurements of ground deformation could be included not only as a joint inversion but also to help constrain initial parameters for modelling the melt fraction and temperature distributions. The cyclic expansion of lava domes gives insight into melt emplacement rates in the upper crust and subsequent subsidence provides information on cooling rates of the upper 100 metres of the volcanic plumbing system. This information would help constrain lithological structure which in turn would provide tighter constraints on the parameters used for thermo-mechanical modelling.

In addition, broad scale InSAR observations of strain gradients, on the scale of kilometres, would provide more detailed information on the emplacement rate of melt in the mush reservoirs beneath active volcanoes. In the case of Montserrat this knowledge could be used to provide a more accurate thermo-mechanical model of the spatial distribution of melt fraction. The periodic collection of InSAR data could also be used to provide a constraint on the temporal evolution of melt fraction distribution. At the Soufrière Hills Volcano, InSAR has already been used to observe the temporal variability in sub-volcanic magma fluxes (Wadge et al., 2006). Future work could include this information to produce

a velocity field from a thermo-mechanical model which incorporates more realistic patterns of melt emplacement in the shallow crust.

Appendix

Diffusion Check

It has been determined that the conversion of the 1D thermo-mechanical modelling results for the spatio-temporal evolution of melt distribution in the shallow crust into a 2D profile for the estimation of a seismic velocity profile has resulted in an underestimation of the lateral extent of diffusion in the model. The following work attempts to address this problem and estimates the magnitude of the underestimation of heat diffusion away from the centre of the zone of sill emplacements in the model.

Problem formulation:

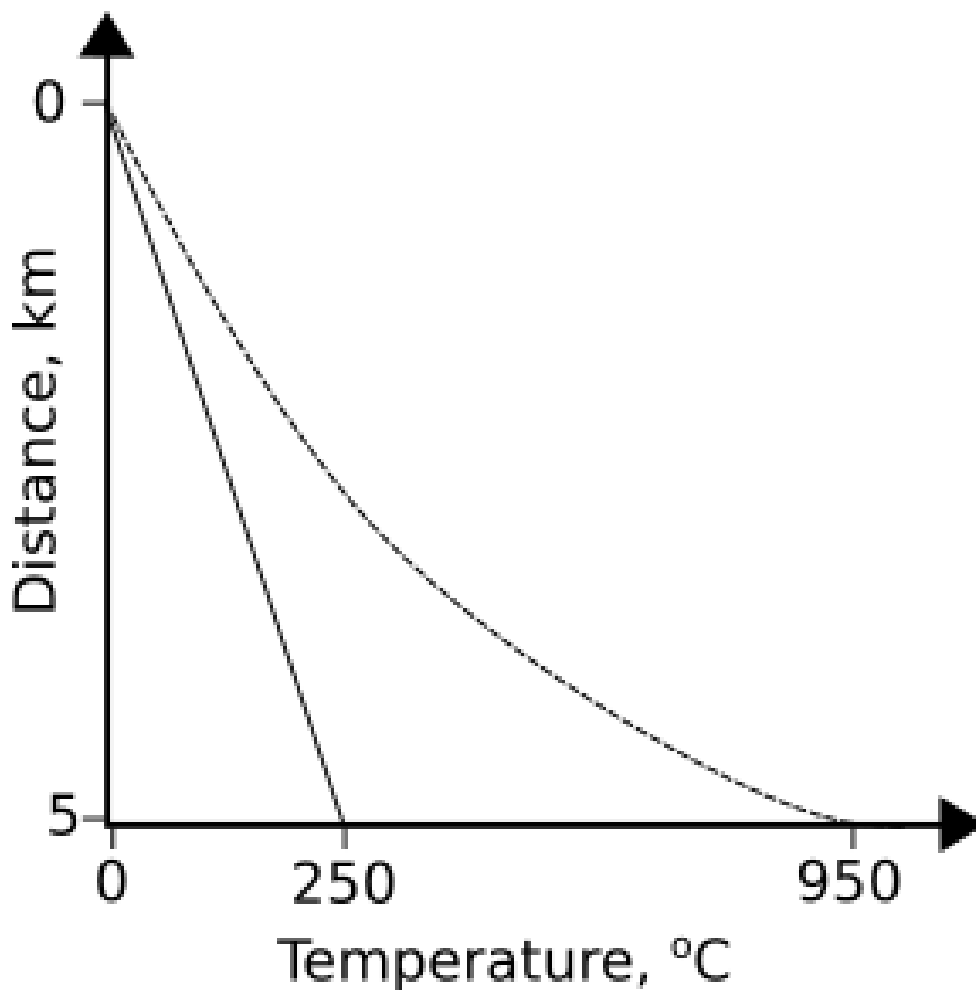


Figure .2: Schematic of the temperature diffusion gradient to be solved. Drawing is not to scale. The solid line shows the geotherm at 50 Kkm⁻¹ while the dashed line shows the gradient produced by the emplacement of heat as sills after 23 ka residence time.

First we will solve an analogous problem:

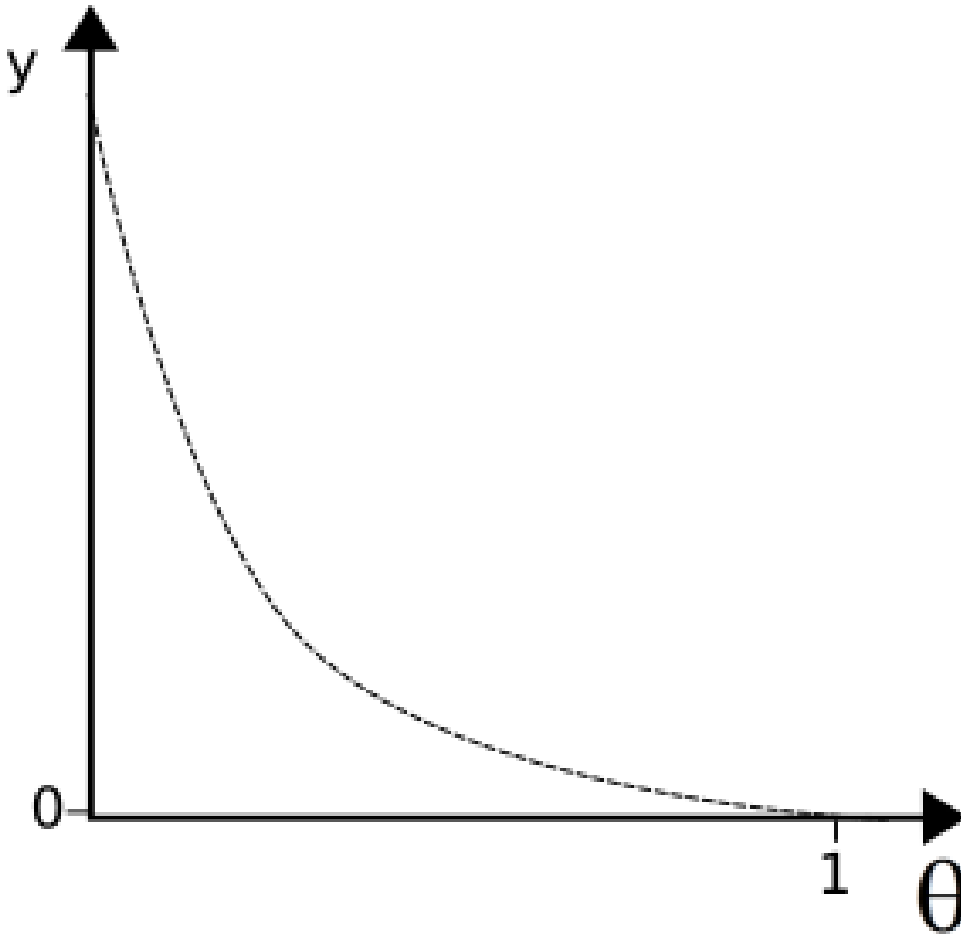


Figure .3: Schematic of the analogous diffusion gradient problem to be solved. Drawing is not to scale.

Our boundary conditions are as follows:

$$\theta = 1 \quad \text{when} \quad y = 0, \quad t \geq 0 \quad (.1)$$

$$\theta = 0 \quad \text{when} \quad y > 0, \quad t = 0 \quad (.2)$$

$$\theta \rightarrow 0 \quad \text{as} \quad y \rightarrow \infty \quad (.3)$$

$$\theta \rightarrow 1 \quad \text{as} \quad t \rightarrow \infty \quad (.4)$$

The diffusion equation, taken from Carslaw and Jaeger (1959) can be written out in terms of θ as follows:

$$\frac{\partial \theta}{\partial t} = \kappa \frac{\partial^2 \theta}{\partial y^2} \quad (.5)$$

where we define κ , from Carslaw and Jaeger (1959) as:

$$\kappa = \frac{k}{C_p \rho} \quad (.6)$$

We then do a transformation of the variables:

$$s = \frac{y}{2\sqrt{\kappa t}} \quad (.7)$$

Since $\sqrt{\kappa t}$ is the only scale length in the problem, so the solution cannot depend on y and t separately.

We substitute in and use the chain rule to get:

$$\frac{\partial \theta}{\partial t} = \frac{d\theta}{ds} \frac{\partial s}{\partial t} = \frac{-s}{2t} \frac{d\theta}{ds} \quad (.8)$$

$$\frac{\partial^2 \theta}{\partial y^2} = \frac{d^2 \theta}{ds^2} \left(\frac{ds}{dy} \right)^2 = \frac{1}{4\kappa t} \frac{d^2 \theta}{ds^2} \quad (.9)$$

Which means that equation .5 becomes:

$$-2s \frac{d\theta}{ds} = \frac{d^2 \theta}{ds^2} \quad (.10)$$

We have converted a PDE to an ODE. This can be solved using integration.

Let $\phi = \frac{d\theta}{ds}$

So now we have

$$-2s\phi = \frac{d\phi}{ds} \quad (.11)$$

Whose solution is:

$$\phi = ce^{-s^2} = \frac{d\theta}{ds} \quad (.12)$$

Where c is the constant of integration. So we integrate again to get:

$$\theta = d + c \int_0^s e^{-\sigma^2} d\sigma \quad (.13)$$

Where d is the second constant of integration and σ is a dummy variable. The limits of the integration will give the value of $\theta(s)$.

We have said from equation .1 that $\theta = 1$ when $y = 0$, so $d = 1$

$$\theta = 1 + c \int_0^s e^{-\sigma^2} d\sigma \quad (.14)$$

And from equation .3, $\theta \rightarrow 0$ as $y \rightarrow \infty$, so $s = \infty$

So:

$$0 = 1 + c \int_0^\infty e^{-\sigma^2} d\sigma \quad (.15)$$

Where the integral is the standard integral $= \sqrt{\frac{\pi}{2}}$, so equation .15 becomes

$$0 = 1 + c\sqrt{\frac{\pi}{2}} \quad (.16)$$

Therefore the constant of integration, $c = -\frac{2}{\sqrt{\pi}}$ and we can now say for θ :

$$\theta = 1 - \frac{2}{\sqrt{\pi}} \int_0^s e^{-\sigma^2} d\sigma \quad (.17)$$

Where the second term on the right hand side of equation .18 is called the error function, which is written $erf(s)$. The error function has no analytical solution but is tabulated.

So we can now use this to figure out how far a thermal anomaly would extend.

Define the thickness of the thermal boundary layer, h , as the distance where $\theta = 0.1$, i.e. the temperature deviation is 10% of the maximum.

From equation .18

$$0.1 = 1 - erf(s) \quad (.18)$$

And from tables of the error function, this gives $s = 1.16$

Because, from equation .7, $s = \frac{y}{2\sqrt{\kappa t}}$ so $1.16 = \frac{h}{2\sqrt{\kappa t}}$ we see $h = 2.32\sqrt{\kappa t}$

Now, going back to the original problem, using figure 4.7 of the thesis where the vertical and lateral temperature gradients are easily comparable; we have a sill intrusion zone with sills being injected at 5km below sea level which marks the top of the zone. The original geotherm is 50^0 Ckm^{-1} , which gives an initial temperature at this depth of 250^0 Ckm^{-1} and a temperature difference of 700^0 Ckm^{-1} for sills intruded at 1223 K, or 950^0 Ckm^{-1} over a time scale of $t = 23 \text{ ka} = 7.3 \times 10^{11} \text{ seconds}$.

Substitute into equation .6 the values for the country rock through which the heat is diffusing, values taken to be the same as the amphibolite used by Paulatto et al. (2012):

$$k = 3 \text{ Js}^{-1}\text{m}^{-1}\text{K}^{-1}, C_p = 1000 \text{ Jkg}^{-1}\text{K}^{-1}, \rho = 2500 \text{ kgm}^{-3},$$

Which gives $\kappa = 1.2 \times 10^{-6} \text{ m}^2\text{s}^{-1}$

So $h = 2.32\sqrt{\kappa t}$, substituting in from above gives:

$$h = 2160\text{m} \quad (3sf)$$

Looking at figure 4.7 in my thesis it can be seen that the vertical distance over which heat has diffused to 10% of its maximum (a 70°C deviation from the original geotherm) is over 2000 metres. This is because at a depth of 3 km below sea level (4 km on the absolute scale in figure 4.7), the temperature is approximately 220°C whereas from the original geotherm it would have been at 150°C . Therefore, as can be seen from the calculation for h , the vertical heat diffusion distance is well estimated in the model adapted from Jackson et al. (2018) and Solano et al. (2012, 2014). The modelled system does not lose heat through the upper boundary layer at a faster rate than would be expected suggesting that the sub volcanic systems are at the correct temperatures within the modelled 1D emplacement zones.

Using the same calculation, we can see that the lateral distance over which heat is shown to diffuse has been underestimated in figure 4.7. The diffusion distance calculated for the horizontal calculation over the run time of the model has been taken from Carslaw and Jaeger (1959). It is important to note that the lateral diffusion distance does not affect the final spatio-temporal distribution of melt that

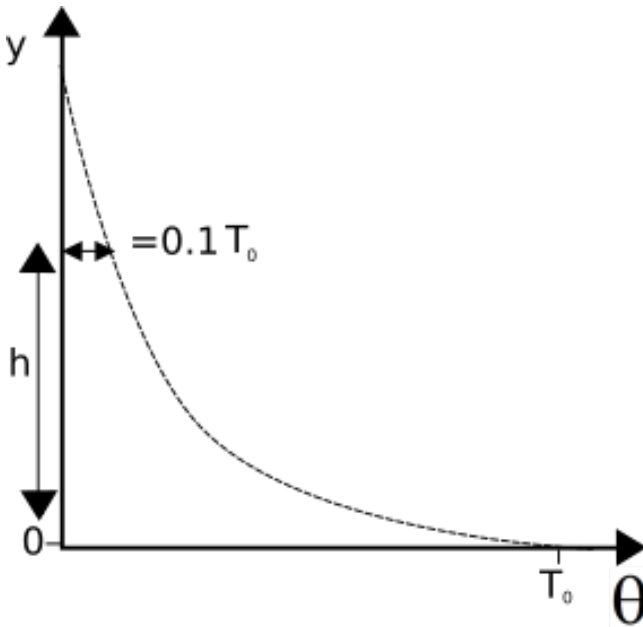


Figure .4: Schematic of the analogous diffusion gradient problem being solved. Drawing is not to scale.

was predicted by the 1D thermo-mechanical model. The 2D extrapolation was simply used to produce a viable, working estimate for a 2D profile over which the calculations for elastic moduli and seismic velocities could be carried out. An extension into 2D modelling is still an on-going process and work is being carried out on the thermo-mechanical model to produce a full 2D cylindrically symmetrical model.

The sharper boundaries produced on the edge of the emplacement zones in the velocity profiles would cause them to be harder to detect using both the FWI and refraction travel time tomography that were used in my thesis. If the lateral diffusion had not been underestimated there would have been a more gradual velocity gradient on the edges of the sill emplacement zone which would have improved recovery using both synthetic FWI and the tomo2D travel time tomography software. This further supports the main conclusion that FWI would be capable of resolving the fine-scale velocity structure at active volcanic centres and that studies would not need to go up to the maximum possible inversion frequency in order to produce useful images for the purpose of investigating the dynamics of the shallow crust beneath volcanoes.

Bibliography

- Alfaro, R., Brandsdóttir, B., Rowlands, D. P., White, R. S., and Gudmundsson, M. T. (2007). Structure of the Grímsvötn central volcano under the Vatnajökull icecap, Iceland. *Geophysical Journal International*, 168(2):863–876.
- Annen, C. (2009). From plutons to magma chambers: Thermal constraints on the accumulation of eruptible silicic magma in the upper crust. *Earth and Planetary Science Letters*, 284(3):409–416.
- Annen, C. (2011). Implications of incremental emplacement of magma bodies for magma differentiation, thermal aureole dimensions and plutonism–volcanism relationships. *Tectonophysics*, 500(1):3–10.
- Annen, C., Blundy, J., Leuthold, J., and Sparks, S. (2015). Construction and evolution of igneous bodies: Towards an integrated perspective of crustal magmatism. *Lithos*, 230:206–221.
- Annen, C., Blundy, J., and Sparks, R. (2006). The genesis of intermediate and silicic magmas in deep crustal hot zones. *Journal of Petrology*, 47(3):505–539.
- Annen, C., Paulatto, M., Sparks, R., Minshull, T., and Kiddle, E. (2014). Quantification of the intrusive magma fluxes during magma chamber growth at Soufrière Hills Volcano (Montserrat, Lesser Antilles). *Journal of Petrology*, 55(3):529–548.
- Annen, C., Pichavant, M., Bachmann, O., and Burgisser, A. (2008). Conditions for the growth of a long-lived shallow crustal magma chamber below Mount Pelee volcano (Martinique, Lesser Antilles Arc). *Journal of Geophysical Research: Solid Earth*, 113(B7).
- Annen, C. and Sparks, R. S. J. (2002). Effects of repetitive emplacement of basaltic intrusions on thermal evolution and melt generation in the crust. *Earth and Planetary Science Letters*, 203(3):937–955.

- Aspinall, W., Miller, A., Lynch, L., Latchman, J., Stewart, R., White, R., and Power, J. (1998). Soufrière Hills eruption, Montserrat, 1995–1997: Volcanic earthquake locations and fault plane solutions. *Geophysical Research Letters*, 25(18):3397–3400.
- Atherton, M. P. (1993). Granite magmatism. *Journal of the Geological Society*, 150(6):1009–1023.
- Bachmann, O. and Bergantz, G. W. (2004). On the origin of crystal-poor rhyolites: extracted from batholithic crystal mushes. *Journal of Petrology*, 45(8):1565–1582.
- Bachmann, O. and Bergantz, G. W. (2006). Gas percolation in upper-crustal silicic crystal mushes as a mechanism for upward heat advection and rejuvenation of near-solidus magma bodies. *Journal of Volcanology and Geothermal research*, 149(1):85–102.
- Bachmann, O. and Bergantz, G. W. (2008). Rhyolites and their source mushes across tectonic settings. *Journal of Petrology*, 49(12):2277–2285.
- Barclay, J., Rutherford, M. J., Carroll, M., Murphy, M., Devine, J., Gardner, J., and Sparks, R. (1998). Experimental phase equilibria constraints on pre-eruptive storage conditions of the Soufrière Hills magma. *Geophysical Research Letters*, 25(18):3437–3440.
- Bargen, N. and Waff, H. S. (1986). Permeabilities, interfacial areas and curvatures of partially molten systems: results of numerical computations of equilibrium microstructures. *Journal of Geophysical Research: Solid Earth*, 91(B9):9261–9276.
- Batzle, M. L., Han, D.-H., and Hofmann, R. (2006). Fluid mobility and frequency-dependent seismic velocity direct measurements. *Geophysics*, 71(1):N1–N9.
- Behr, G. E. and Schroeder, L. H. (1942). Process for purifying metals. US Patent 2,296,196.
- Bergantz, G. W. (1989). Underplating and partial melting: implications for melt generation and extraction. *Science*, 245(4922):1093–1095.
- Bergantz, G. W. and Dawes, R. (1994). Aspects of magma generation and ascent in continental lithosphere. *International Geophysics*, 57:291–317.
- Bergman, D. J. (1978). The dielectric constant of a composite material - a problem in classical physics. *Physics Reports*, 43(9):377–407.
- Berryman, J. G. (1980a). Long-wavelength propagation in composite elastic media I. Spherical inclusions. *The Journal of the Acoustical Society of America*, 68(6):1809–1819.
- Berryman, J. G. (1980b). Long-wavelength propagation in composite elastic media II. Ellipsoidal inclusions. *The Journal of the Acoustical Society of America*, 68(6):1820–1831.

- Berryman, J. G. (1985). Scattering by a spherical inhomogeneity in a fluid-saturated porous medium. *Journal of mathematical physics*, 26(6):1408–1419.
- Berryman, J. G. (1990). Stable iterative reconstruction algorithm for nonlinear traveltime tomography. *Inverse problems*, 6(1):21.
- Berryman, J. G. (1995). Mixture theories for rock properties. *Rock physics & phase relations: A handbook of physical constants*, pages 205–228.
- Berryman, J. G. (2005). Bounds and self-consistent estimates for elastic constants of random polycrystals with hexagonal, trigonal, and tetragonal symmetries. *Journal of the Mechanics and Physics of Solids*, 53(10):2141–2173.
- Berryman, J. G. and Berge, P. A. (1993). Rock elastic properties: dependence on microstructure. *ASME APPLIED MECHANICS DIVISION-PUBLICATIONS-AMD*, 166:1–1.
- Berryman, J. G. and Berge, P. A. (1996). Critique of two explicit schemes for estimating elastic properties of multiphase composites. *Mechanics of Materials*, 22(2):149–164.
- Berryman, J. G. and Milton, G. W. (1991). Exact results for generalized Gassmann’s equations in composite porous media with two constituents. *Geophysics*, 56(12):1950–1960.
- Birch, F. (1961). The velocity of compressional waves in rocks to 10 kilobars: 2. *Journal of Geophysical Research*, 66(7):2199–2224.
- Blundy, J. and Cashman, K. V. (2001). Ascent-driven crystallisation of dacite magmas at Mount St. Helens, 1980-1986. *Contributions to Mineralogy and Petrology*, 140:631–650.
- Blundy, J. and Cashman, K. V. (2008). Petrologic reconstruction of magmatic system variables and processes. *Reviews in Mineralogy and Geochemistry*, 69:179–239.
- Bouska, J. (2008). Advantages of wide-patch, wide-azimuth ocean-bottom seismic reservoir surveillance. *The Leading Edge*, 27(12):1662–1681.
- Bowen, N. (1922). The reaction principle in petrogenesis. *The Journal of Geology*, 30(3):177–198.
- Bowen, N. L. (1915a). Crystallization-differentiation in silicate liquids. *American Journal of Science*, 230(230):175–191.
- Bowen, N. L. (1915b). The later stages of the evolution of the igneous rocks. *The Journal of Geology*, 23(S8):1–91.

- Bowen, N. L. (1945). Phase equilibria bearing on the origin and differentiation of alkaline rocks. *American Journal of Science*, 243:75–89.
- Boynnton, C., Westbrook, G., Bott, M., and Long, R. (1979). A seismic refraction investigation of crustal structure beneath the Lesser Antilles island arc. *Geophysical Journal International*, 58(2):371–393.
- Brandeis, G. and Marsh, B. D. (1989). The convective liquidus in a solidifying magma chamber: a fluid dynamic investigation. *Nature*, 339(6226):613–616.
- Brandsdóttir, B., Menke, W., Einarsson, P., White, R. S., and Staples, R. K. (1997). Färoe-Iceland Ridge Experiment 2. Crustal structure of the Krafla central volcano. *Journal of Geophysical Research: Solid Earth*, 102(B4):7867–7886.
- Brenders, A. and Pratt, R. (2007). Full waveform tomography for lithospheric imaging: Results from a blind test in a realistic crustal model. *Geophysical Journal International*, 168(1):133–151.
- Brocher, T. M. (2005). Empirical relations between elastic wave speeds and density in the Earth’s crust. *Bulletin of the Seismological Society of America*, 95(6):2081–2092.
- Brown, M. (1994). The generation, segregation, ascent and emplacement of granite magma: the migmatite-to-crustally-derived granite connection in thickened orogens. *Earth-Science Reviews*, 36(1-2):83–130.
- Bruggeman, D. (1935). Effective medium approximations. *Ann. Phys*, 24:636–664.
- Budiansky, B. and O’Connell, R. J. (1976). Elastic moduli of a cracked solid. *International journal of Solids and structures*, 12(2):81–97.
- Byerly, K., Brown, L., Voight, B., and Miller, V. (2010). Reflection imaging of deep structure beneath Montserrat using microearthquake sources. *Geophysical Research Letters*, 37(19).
- Calvert, A. J., Klemperer, S. L., Takahashi, N., and Kerr, B. C. (2008). Three-dimensional crustal structure of the Mariana island arc from seismic tomography. *Journal of Geophysical Research: Solid Earth*, 113(B1).
- Caricchi, L. and Blundy, J. (2015a). Experimental petrology of monotonous intermediate magmas. *Geological Society, London, Special Publications*, 422(1):105–130.
- Caricchi, L. and Blundy, J. (2015b). The temporal evolution of chemical and physical properties of magmatic systems. *Geological Society, London, Special Publications*, 422(1):1–15.

- Caristan, Y. (1982). The transition from high temperature creep to fracture in Maryland diabase. *Journal of Geophysical Research: Solid Earth*, 87(B8):6781–6790.
- Carslaw, H. S. and Jaeger, J. C. (1959). Conduction of heat in solids. *Oxford: Clarendon Press, 1959, 2nd ed.*
- Cashman, K. and Blundy, J. (2013). Petrological cannibalism: the chemical and textural consequences of incremental magma body growth. *Contributions to Mineralogy and Petrology*, 166(3):703–729.
- Cashman, K. V. and Giordano, G. (2014). Calderas and magma reservoirs. *Journal of Volcanology and Geothermal Research*, 288:28–45.
- Cashman, K. V., Sparks, R. S. J., and Blundy, J. D. (2017). Vertically extensive and unstable magmatic systems: A unified view of igneous processes. *Science*, 355(6331):eaag3055.
- Chang, W.-L., Smith, R. B., Wicks, C., Farrell, J. M., and Puskas, C. M. (2007). Accelerated uplift and magmatic intrusion of the Yellowstone caldera, 2004 to 2006. *Science*, 318(5852):952–956.
- Chappell, B. and White, A. J. R. (2001). Two contrasting granite types: 25 years later. *Australian Journal of Earth Sciences*, 48(4):489–499.
- Chappell, B. W., White, A., Williams, I., and Wyborn, D. (2004). Low-and high-temperature granites. *Earth and Environmental Science Transactions of the Royal Society of Edinburgh*, 95(1-2):125–140.
- Cheadle, M., Elliott, M., and McKenzie, D. (2004). Percolation threshold and permeability of crystallizing igneous rocks: The importance of textural equilibrium. *Geology*, 32(9):757–760.
- Cheadle, M., McGeary, S., Warner, M., and Matthews, D. (1987). Extensional structures on the western UK continental shelf: a review of evidence from deep seismic profiling. *Geological Society, London, Special Publications*, 28(1):445–465.
- Chironi, C., Morgan, J., and Warner, M. (2006). Imaging of intrabasalt and subbasalt structure with full wavefield seismic tomography. *Journal of Geophysical Research: Solid Earth*, 111(B5).
- Chopelas, A. (1992). Sound velocities of MgO to very high compression. *Earth and planetary science letters*, 114(1):185–192.
- Chopelas, A. and Boehler, R. (1989). Thermal expansion measurements at very high pressure, systematics, and a case for a chemically homogeneous mantle. *Geophysical Research Letters*, 16(11):1347–1350.
- Chopelas, A. and Boehler, R. (1992). Thermal expansivity in the lower mantle. *Geophysical Research Letters*, 19(19):1983–1986.

- Christensen, N. I. (1974). Compressional wave velocities in possible mantle rocks to pressures of 30 kilobars. *Journal of Geophysical Research*, 79(2):407–412.
- Christensen, N. I. and Mooney, W. D. (1995). Seismic velocity structure and composition of the continental crust: A global view. *Journal of Geophysical Research: Solid Earth*, 100(B6):9761–9788.
- Christeson, G. L., Mann, P., Escalona, A., and Aitken, T. J. (2008). Crustal structure of the Caribbean Northeastern South America arc-continent collision zone. *Journal of Geophysical Research: Solid Earth*, 113(B8).
- Chung, D. and Buessem, W. (1967). The Voigt-Reuss-Hill Approximation and Elastic Moduli of Polycrystalline MgO, CaF₂, β -ZnS, ZnSe, and CdTe. *Journal of Applied Physics*, 38(6):2535–2540.
- Clarke, D. B. (1992). *Granitoid rocks*, volume 7. Springer Science & Business Media.
- Clemens, J. (2003). S-type granitic magmas petrogenetic issues, models and evidence. *Earth-Science Reviews*, 61(1):1–18.
- Clemens, J. and Mawer, C. (1992). Granitic magma transport by fracture propagation. *Tectonophysics*, 204(3-4):339–360.
- Coleman, D. S., Glazner, A. F., Miller, J., Bradford, K., Frost, T., Joye, J., and Bachl, C. (1995). Exposure of a Late Cretaceous layered mafic-felsic magma system in the central Sierra Nevada Batholith, California. *Contributions to Mineralogy and Petrology*, 120(2):129–136.
- Coleman, D. S., Gray, W., and Glazner, A. F. (2004). Rethinking the emplacement and evolution of zoned plutons: Geochronologic evidence for incremental assembly of the Tuolumne Intrusive Suite, California. *Geology*, 32(5):433–436.
- Collier, J. and Singh, S. (1997). Detailed structure of the top of the melt body beneath the East Pacific Rise at 9 40° N from waveform inversion of seismic reflection data. *Journal of Geophysical Research: Solid Earth*, 102(B9):20287–20304.
- Comeau, M. J., Unsworth, M. J., Ticona, F., and Sunagua, M. (2015). Magnetotelluric images of magma distribution beneath Volcán Uturuncu, Bolivia: Implications for magma dynamics. *Geology*, 43(3):243–246.
- Connolly, J. and Podladchikov, Y. Y. (1998). Compaction-driven fluid flow in viscoelastic rock. *Geodinamica Acta*, 11(2-3):55–84.

- Cook, F. A. (2002). Fine structure of the continental reflection Moho. *Geological Society of America Bulletin*, 114(1):64–79.
- Cooper, K. M. and Kent, A. J. (2014). Rapid remobilization of magmatic crystals kept in cold storage. *Nature*, 506(7489):480–483.
- Cooper, R. and Kohlstedt, D. (1984). Solution-precipitation enhanced diffusional creep of partially molten olivine-basalt aggregates during hot-pressing. *Tectonophysics*, 107(3-4):207–233.
- Couch, S., Sparks, R., and Carroll, M. (2003). The kinetics of degassing-induced crystallization at Soufrière Hills Volcano, Montserrat. *Journal of Petrology*, 44(8):1477–1502.
- Courant, R., Friedrichs, K., and Lewy, H. (1928). Über die partiellen Differenzengleichungen der mathematischen Physik. *Mathematische annalen*, 100(1):32–74.
- Cruden, A. R. (1998). On the emplacement of tabular granites. *Journal of the Geological Society-London*, 155(5):853–862.
- Daly, R. A. (1914). *Igneous rocks and their origin*. McGraw-Hill book company, inc.
- Davis, R. H. and Acrivos, A. (1985). Sedimentation of noncolloidal particles at low Reynolds numbers. *Annual Review of Fluid Mechanics*, 17(1):91–118.
- Davy, R., Morgan, J. V., Minshull, T., Bayrakci, G., Bull, J., Klaeschen, D., Reston, T., Sawyer, D. S., Lymer, G., and Cresswell, D. (2017). Resolving the fine-scale velocity structure of continental hyperextension at the Deep Galicia Margin using full-waveform inversion. *Geophysical Journal International*, 212(1):244–263.
- DeBari, S. M. and Coleman, R. (1989). Examination of the deep levels of an island arc: Evidence from the Tonsina Ultramafic-Mafic Assemblage, Tonsina, Alaska. *Journal of Geophysical Research: Solid Earth*, 94(B4):4373–4391.
- Devine, J., Murphy, M., Rutherford, M., Barclay, J., Sparks, R., Carroll, M., Young, S., and Gardner, J. (1998). Petrologic evidence for pre-eruptive pressure-temperature conditions, and recent reheating, of andesitic magma erupting at the Soufrière Hills Volcano, Montserrat, WI. *Geophysical Research Letters*, 25(19):3669–3672.
- Dufek, J. and Bergantz, G. (2005). Lower crustal magma genesis and preservation: a stochastic framework for the evaluation of basalt–crust interaction. *Journal of Petrology*, 46(11):2167–2195.

- Dunn, R. A., Toomey, D. R., and Solomon, S. C. (2000). Three-dimensional seismic structure and physical properties of the crust and shallow mantle beneath the East Pacific Rise at 9°30'N. *Journal of Geophysical Research: Solid Earth*, 105(B10):23537–23555.
- Dziewonski, A. M. and Anderson, D. L. (1981). Preliminary reference Earth model. *Physics of the earth and planetary interiors*, 25(4):297–356.
- Eberhart-Phillips, D., Han, D.-H., and Zoback, M. D. (1989). Empirical relationships among seismic velocity, effective pressure, porosity, and clay content in sandstone. *Geophysics*, 54(1):82–89.
- Flügelner, M. M. and White, R. S. (2001). Seismic structure of basalt flows from surface seismic data, borehole measurements, and synthetic seismogram modeling. *Geophysics*, 66(6):1925–1936.
- Foden, J. and Green, D. (1992). Possible role of amphibole in the origin of andesite: some experimental and natural evidence. *Contributions to Mineralogy and Petrology*, 109(4):479–493.
- Foroozan, R., Elsworth, D., Voight, B., and Mattioli, G. S. (2010). Dual reservoir structure at Soufrière Hills Volcano inferred from continuous GPS observations and heterogeneous elastic modeling. *Geophysical Research Letters*, 37(19).
- Fruehn, J., Flügelner, M. M., and White, R. S. (2001). Integrated wide-angle and near-vertical subbasalt study using large-aperture seismic data from the Faeroe-Shetland region. *Geophysics*, 66(5):1340–1348.
- Galgana, G. A., McGovern, P. J., and Grosfils, E. B. (2011). Evolution of large Venusian volcanoes: Insights from coupled models of lithospheric flexure and magma reservoir pressurization. *Journal of Geophysical Research: Planets*, 116(E3).
- Gassmann, F. (1951a). Elastic waves through a packing of spheres. *Geophysics*, 16(4):673–685.
- Gassmann, F. (1951b). Elasticity of porous media. *Vierteljahrsschrift der Naturforschenden Gesellschaft*, 96:1–23.
- Glazner, A. F. (1994). Foundering of mafic plutons and density stratification of continental crust. *Geology*, 22(5):435–438.
- Glazner, A. F. and Bartley, J. M. (2006). Is stopping a volumetrically significant pluton emplacement process? *Geological Society of America Bulletin*, 118(9-10):1185–1195.
- Glazner, A. F., Bartley, J. M., Coleman, D. S., Gray, W., and Taylor, R. Z. (2004). Are plutons assembled over millions of years by amalgamation from small magma chambers? *GSA today*, 14(4/5):4–12.

- Glazner, A. F. and Miller, D. M. (1997). Late-stage sinking of plutons. *Geology*, 25(12):1099–1102.
- Gualda, G. A. and Ghiorso, M. S. (2013). The Bishop Tuff giant magma body: an alternative to the Standard Model. *Contributions to Mineralogy and Petrology*, 166(3):755–775.
- Gutenberg, B. (1914). Ueber Erdbebenwellen. VII A. Beobachtungen an Registrierungen von Fernbeben in Göttingen und Folgerung über die Konstitution des Erdkörpers (mit Tafel). *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, 1914:125–176.
- Haas, A. and Dubrule, O. (1994). Geostatistical inversion—a sequential method of stochastic reservoir modelling constrained by seismic data. *Firstbreak*, 12(11):561–569.
- Halliday, A., Mahood, G. A., Holden, P., Metz, J., Dempster, T., and Davidson, J. P. (1989). Evidence for long residence times of rhyolitic magma in the Long Valley magmatic system: the isotopic record in precaldera lavas of Glass Mountain. *Earth and Planetary Science Letters*, 94(3-4):274–290.
- Halliday, A., Stephens, W., and Harmon, R. (1980). Rb-Sr and O isotopic relationships in 3 zoned Caledonian granitic plutons, Southern Uplands, Scotland: evidence for varied sources and hybridization of magmas. *Journal of the Geological Society*, 137(3):329–348.
- Han, D.-h. and Batzle, M. L. (2004). Gassmann’s equation and fluid-saturation effects on seismic velocities. *Geophysics*, 69(2):398–405.
- Hansen, T. M., Singh, S. C., and Jacobsen, B. H. (1999). Sensitivity of seismic wide-angle wave-field and first arrival times to fine scale crustal structure and moho topography. *Geophysical research letters*, 26(16):2573–2576.
- Hanson, R. B. and Glazner, A. F. (1995). Thermal requirements for extensional emplacement of granitoids. *Geology*, 23(3):213–216.
- Harford, C., Pringle, M., Sparks, R., and Young, S. (2002). The volcanic evolution of Montserrat using $^{40}\text{Ar}/^{39}\text{Ar}$ geochronology. *Geological Society, London, Memoirs*, 21(1):93–113.
- Harford, C. L. and Sparks, R. S. J. (2001). Recent remobilisation of shallow-level intrusions on Montserrat revealed by hydrogen isotope composition of amphiboles. *Earth and Planetary Science Letters*, 185(3):285–297.
- Harker, A. (1909). *The natural history of igneous rocks*. Macmillan.
- Hashin, Z. (1960). *The elastic moduli of heterogeneous materials*. US Department of Commerce, Office of Technical Services.

- Hashin, Z. and Shtrikman, S. (1961a). Note on a variational approach to the theory of composite elastic materials. *Journal of the Franklin Institute*, 271(4):336–341.
- Hashin, Z. and Shtrikman, S. (1961b). Note on the effective constants of composite materials. *Journal of the Franklin institute*, 271(5):423–426.
- Hashin, Z. and Shtrikman, S. (1962). A variational approach to the theory of the elastic behaviour of polycrystals. *Journal of the Mechanics and Physics of Solids*, 10(4):343–352.
- Hashin, Z. and Shtrikman, S. (1963). A variational approach to the theory of the elastic behaviour of multiphase materials. *Journal of the Mechanics and Physics of Solids*, 11(2):127–140.
- Hautmann, S., Gottsmann, J., Camacho, A. G., Fournier, N., Sacks, I. S., and Sparks, R. S. J. (2010a). Mass variations in response to magmatic stress changes at Soufrière Hills Volcano, Montserrat (WI): Insights from 4-D gravity data. *Earth and Planetary Science Letters*, 290(1):83–89.
- Hautmann, S., Gottsmann, J., Sparks, R. S. J., Mattioli, G. S., Sacks, I. S., and Strutt, M. H. (2010b). Effect of mechanical heterogeneity in arc crust on volcano deformation with application to Soufrière Hills Volcano, Montserrat, West Indies. *Journal of Geophysical Research: Solid Earth*, 115(B9).
- Hawkesworth, C., George, R., Turner, S., and Zellmer, G. (2004). Time scales of magmatic processes. *Earth and Planetary Science Letters*, 218(1):1–16.
- Hill, R. (1952). The elastic behaviour of a crystalline aggregate. *Proceedings of the Physical Society. Section A*, 65(5):349.
- Hill, R. (1963). Elastic properties of reinforced solids: some theoretical principles. *Journal of the Mechanics and Physics of Solids*, 11(5):357–372.
- Hill, R. (1965). A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, 13(4):213–222.
- Hobro, J. W., Singh, S. C., and Minshull, T. A. (2003). Three-dimensional tomographic inversion of combined reflection and refraction seismic traveltime data. *Geophysical Journal International*, 152(1):79–93.
- Hole, J., Zelt, C., and Pratt, R. (2005). Advances in controlled-source seismic imaging. *Eos, Transactions American Geophysical Union*, 86(18):177–181.
- Humphreys, M. C., Christopher, T., and Hards, V. (2009). Microlite transfer by disaggregation of mafic inclusions following magma mixing at Soufrière Hills Volcano, Montserrat. *Contributions to Mineralogy and Petrology*, 157(5):609–624.

- Huppert, H. E. and Sparks, R. S. J. (1988a). Melting the roof of a chamber containing a hot, turbulently convecting fluid. *Journal of Fluid Mechanics*, 188:107–131.
- Huppert, H. E. and Sparks, R. S. J. (1988b). The generation of granitic magmas by intrusion of basalt into continental crust. *Journal of Petrology*, 29(3):599–624.
- Ingham, D. B. and Pop, I. (1998). *Transport phenomena in porous media*. Elsevier.
- Isaak, D. G. (1992). High-temperature elasticity of iron-bearing olivines. *Journal of Geophysical Research: Solid Earth*, 97(B2):1871–1885.
- Jackson, M., Blundy, J., and Sparks, R. (2018). Reactive Melt Flow in Mush Reservoirs: A Key Process Controlling Storage and Differentiation of Magma in the Continental Crust. *AGU Fall Meeting*, December(Chemistry, Mechanics, Geophysics, and Timescales of Magmatic Processes):na.
- Jackson, M., Gallagher, K., Petford, N., and Cheadle, M. (2005). Towards a coupled physical and chemical model for tonalite–trondhjemite–granodiorite magma formation. *Lithos*, 79(1):43–60.
- Jackson, M. D., Cheadle, M. J., and Atherton, M. P. (2003). Quantitative modeling of granitic melt generation and segregation in the continental crust. *Journal of Geophysical Research: Solid Earth*, 108(B7).
- Jellinek, A. M. and DePaolo, D. J. (2003). A model for the origin of large silicic magma chambers: precursors of caldera-forming eruptions. *Bulletin of Volcanology*, 65(5):363–381.
- Jellinek, A. M. and Kerr, R. C. (1999). Mixing and compositional stratification produced by natural convection: 2. Applications to the differentiation of basaltic and silicic magma chambers and komatiite lava flows. *Journal of Geophysical Research: Solid Earth*, 104(B4):7203–7218.
- Kamei, R., Pratt, R. G., and Tsuji, T. (2012). Waveform tomography imaging of a megasplay fault system in the seismogenic Nankai subduction zone. *Earth and Planetary Science Letters*, 317:343–353.
- Kanamori, H. and Anderson, D. L. (1977). Importance of physical dispersion in surface wave and free oscillation problems. *Reviews of Geophysics*, 15(1):105–112.
- Kapoor, S., Vigh, D., Wiarda, E., and Alwon, S. (2013). Full waveform inversion around the world. In *75th EAGE Conference & Exhibition incorporating SPE EUROPEC 2013*.
- Karato, S.-i. (1993). Importance of anelasticity in the interpretation of seismic tomography. *Geophysical Research Letters*, 20(15):1623–1626.

- Karato, S.-i. and Karki, B. B. (2001). Origin of lateral variation of seismic wave velocities and density in the deep mantle. *Journal of Geophysical Research: Solid Earth*, 106(B10):21771–21783.
- Karato, S.-I. and Spetzler, H. (1990). Defect microdynamics in minerals and solid-state mechanisms of seismic wave attenuation and velocity dispersion in the mantle. *Reviews of Geophysics*, 28(4):399–421.
- Katz, R. F. (2008). Magma dynamics with the enthalpy method: Benchmark solutions and magmatic focusing at mid-ocean ridges. *Journal of Petrology*, 49(12):2099–2121.
- Kay, R. W. and Kay, S. M. (1993). Delamination and delamination magmatism. *Tectonophysics*, 219(1-3):177–189.
- Kelemen, P. B., Shimizu, N., and Salters, V. J. (1995a). Extraction of mid-ocean-ridge basalt from the upwelling mantle by focused flow of melt in dunite channels. *Nature*, 375(6534):747–753.
- Kelemen, P. B., Whitehead, J., Aharonov, E., and Jordahl, K. A. (1995b). Experiments on flow focusing in soluble porous media, with applications to melt extraction from the mantle. *Journal of Geophysical Research: Solid Earth*, 100(B1):475–496.
- Kellogg, L. H., Hager, B. H., and Van Der Hilst, R. D. (1999). Compositional stratification in the deep mantle. *Science*, 283(5409):1881–1884.
- Kenedi, C., Sparks, R., Malin, P., Voight, B., Dean, S., Minshull, T., Paulatto, M., Peirce, C., and Shalev, E. (2010). Contrasts in morphology and deformation offshore Montserrat: New insights from the SEA-CALIPSO marine cruise data. *Geophysical Research Letters*, 37(19).
- Kiddle, E., Edwards, B., Loughlin, S., Petterson, M., Sparks, R., and Voight, B. (2010). Crustal structure beneath Montserrat, Lesser Antilles, constrained by xenoliths, seismic velocity structure and petrology. *Geophysical Research Letters*, 37(19).
- Kiddle, E. J. (2011). *The structure of the crust and magmatic system at Montserrat, Lesser Antilles*. PhD thesis, University of Bristol.
- Klügel, A., Hansteen, T. H., and Galipp, K. (2005). Magma storage and underplating beneath Cumbre Vieja volcano, la Palma (Canary Islands). *Earth and Planetary Science Letters*, 236(1):211–226.
- Kodaira, S., Sato, T., Takahashi, N., Ito, A., Tamura, Y., Tatsumi, Y., and Kaneda, Y. (2007a). Seismological evidence for variable growth of crust along the Izu intraoceanic arc. *Journal of Geophysical Research: Solid Earth*, 112(B5).

- Kodaira, S., Sato, T., Takahashi, N., Miura, S., Tamura, Y., Tatsumi, Y., and Kaneda, Y. (2007b). New seismological constraints on growth of continental crust in the Izu-Bonin intra-oceanic arc. *Geology*, 35(11):1031–1034.
- Korenaga, J., Holbrook, W., Kent, G., Kelemen, P., Detrick, R., Larsen, H.-C., Hopper, J., and Dahl-Jensen, T. (2000). Crustal structure of the southeast Greenland margin from joint refraction and reflection seismic tomography. *Journal of Geophysical Research: Solid Earth*, 105(B9):21591–21614.
- Korenaga, J., Holbrook, W. S., Detrick, R. S., and Kelemen, P. B. (2001). Gravity anomalies and crustal structure at the southeast Greenland margin. *Journal of Geophysical Research: Solid Earth*, 106(B5):8853–8870.
- Korenaga, J., Kelemen, P. B., and Holbrook, W. S. (2002). Methods for resolving the origin of large igneous provinces from crustal seismology. *Journal of Geophysical Research: Solid Earth*, 107(B9).
- Kumazawa, M. and Anderson, O. L. (1969). Elastic moduli, pressure derivatives, and temperature derivatives of single-crystal olivine and single-crystal forsterite. *Journal of Geophysical Research*, 74(25):5961–5972.
- Kuster, G. T. and Toksöz, M. N. (1974a). Velocity and attenuation of seismic waves in two-phase media: Part I. Theoretical formulations. *Geophysics*, 39(5):587–606.
- Kuster, G. T. and Toksöz, M. N. (1974b). Velocity and attenuation of seismic waves in two-phase media: Part II. Experimental results. *Geophysics*, 39(5):607–618.
- Le Friant, A., Harford, C., Deplus, C., Boudon, G., Sparks, R., Herd, R., and Komorowski, J. (2004). Geomorphological evolution of Montserrat (West Indies): importance of flank collapse and erosional processes. *Journal of the Geological Society*, 161(1):147–160.
- Le Friant, A., Lock, E., Hart, M., Boudon, G., Sparks, R., Leng, M., Smart, C. W., Komorowski, J.-C., Deplus, C., and Fisher, J. (2008). Late Pleistocene tephrochronology of marine sediments adjacent to Montserrat, Lesser Antilles volcanic arc. *Journal of the Geological Society*, 165(1):279–289.
- Lee, C.-T. A. and Morton, D. M. (2015). High silica granites: Terminal porosity and crystal settling in shallow magma chambers. *Earth and Planetary Science Letters*, 409:23–31.
- Lees, J. M. (2007). Seismic tomography of magmatic systems. *Journal of Volcanology and Geothermal Research*, 167(1):37–56.
- Lehmann, I. (1936). P: Publications du Bureau Central Séismologique International. *A14*, pages 87–115.

- Linde, A. T., Sacks, S., Hidayat, D., Voight, B., Clarke, A., Elsworth, D., Mattioli, G., Malin, P., Shalev, E., Sparks, S., et al. (2010). Vulcanian explosion at Soufrière Hills Volcano, Montserrat on March 2004 as revealed by strain data. *Geophysical Research Letters*, 37(19).
- Lizarralde, D., Holbrook, W. S., McGeary, S., Bangs, N. L., and Diebold, J. B. (2002). Crustal construction of a volcanic arc, wide-angle seismic results from the western Alaska Peninsula. *Journal of Geophysical Research: Solid Earth*, 107(B8).
- Loughlin, S., Luckett, R., Ryan, G., Christopher, T., Hards, V., De Angelis, S., Jones, L., and Strutt, M. (2010). An overview of lava dome evolution, dome collapse and cyclicity at Soufrière Hills Volcano, Montserrat, 2005–2007. *Geophysical Research Letters*, 37(19).
- Lu, M., Hofmann, A. W., Mazzucchelli, M., and Rivalenti, G. (1997). The mafic-ultramafic complex near Finero (Ivrea-Verbano Zone), II. Geochronology and isotope geochemistry. *Chemical Geology*, 140(3-4):223–235.
- Lyell, C. (1833). *Principles of Geology: Being an Attempt to Explain the Former Changes of the Earth's Surface, by Reference to Causes Now in Operation*, volume 3. J. Murray.
- Mackenzie, G., Thybo, H., and Maguire, P. (2005). Crustal velocity structure across the Main Ethiopian Rift: results from two-dimensional wide-angle seismic modelling. *Geophysical Journal International*, 162(3):994–1006.
- Mahood, G. A. and Halliday, A. N. (1988). Generation of high-silica rhyolite: a Nd, Sr, and O isotopic study of Sierra La Primavera, Mexican Neovolcanic Belt. *Contributions to Mineralogy and Petrology*, 100(2):183–191.
- Man, C.-S. and Huang, M. (2011). A simple explicit formula for the Voigt-Reuss-Hill average of elastic polycrystals with arbitrary crystal and texture symmetries. *Journal of Elasticity*, 105(1):29–48.
- Marsh, B. (1978). On the cooling of ascending andesitic magma. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 288(1355):611–625.
- Marsh, B. (1981). On the crystallinity, probability of occurrence, and rheology of lava and magma. *Contributions to Mineralogy and Petrology*, 78(1):85–98.
- Marsh, B. D. (1989). Magma chambers. *Annual Review of Earth and Planetary Sciences*, 17(1):439–472.
- Mattioli, G. S., Dixon, T. H., Farina, F., Howell, E. S., Jansma, P. E., and Smith, A. L. (1998). GPS measurement of surface deformation around Soufrière Hills volcano, Montserrat from October 1995 to July 1996. *Geophysical Research Letters*, 25(18):3417–3420.

- Mattioli, G. S., Herd, R. A., Strutt, M. H., Ryan, G., Widiwijayanti, C., and Voight, B. (2010). Long term surface deformation of Soufrière Hills Volcano, Montserrat from GPS geodesy: Inferences from simple elastic inverse models. *Geophysical Research Letters*, 37(19).
- Mattioli, G. S., Young, S. R., Voight, B., Steven, R., Sparks, J., Shalev, E., Sacks, S., Malin, P., Linde, A., Johnston, W., et al. (2004). Prototype PBO instrumentation of CALIPSO project captures world-record lava dome collapse on Montserrat Volcano. *Eos, Transactions American Geophysical Union*, 85(34):317–325.
- Matzel, J. E., Bowring, S. A., and Miller, R. B. (2006). Time scales of pluton construction at differing crustal levels: Examples from the Mount Stuart and Tenpeak intrusions, North Cascades, Washington. *Geological Society of America Bulletin*, 118(11-12):1412–1430.
- Mavko, G., Mukerji, T., and Dvorkin, J. (2009). *The rock physics handbook: Tools for seismic analysis of porous media*. Cambridge university press.
- Mavko, G. M. (1980). Velocity and attenuation in partially molten rocks. *Journal of Geophysical Research: Solid Earth*, 85(B10):5173–5189.
- McCaffrey, K. and Petford, N. (1997). Are granitic intrusions scale invariant? *Journal of the Geological Society*, 154(1):1–4.
- McKenzie, D. (1984). The generation and compaction of partially molten rock. *Journal of Petrology*, 25(3):713–765.
- McKenzie, D. (1985). The extraction of magma from the crust and mantle. *Earth and Planetary Science Letters*, 74(1):81–91.
- McKenzie, D. (1987). The compaction of igneous and sedimentary rocks. *Journal of the Geological Society*, 144(2):299–307.
- McNutt, S. R. (1996). Seismic monitoring and eruption forecasting of volcanoes: a review of the state-of-the-art and case histories. In *Monitoring and mitigation of volcano hazards*, pages 99–146. Springer.
- McQuillin, R., Bacon, M., and Barclay, W. (1984). *An introduction to seismic interpretation-Reflection seismics in petroleum exploration*. Graham and Trotman Ltd., Gaithersburg, MD.
- Menand, T. (2008). The mechanics and dynamics of sills in layered elastic rocks and their implications for the growth of laccoliths and other igneous complexes. *Earth and Planetary Science Letters*, 267(1):93–99.

- Menke, W. (1984). *Geophysical Data Analysis: Discrete Inverse Theory Academic. New York.*
- Middlemost, E. A. (1991). Towards a comprehensive classification of igneous rocks and magmas. *Earth-Science Reviews*, 31(2):73–87.
- Misaghi, A., Negahban, S., Landrø, M., and Javaherian, A. (2010). A comparison of rock physics models for fluid substitution in carbonate rocks. *Exploration Geophysics*, 41(2):146–154.
- Mogi, K. (1958). *Relations between the eruptions of various volcanoes and the deformations of the ground surfaces around them.*
- Moorkamp, M., Heincke, B., Jegen, M., Roberts, A. W., and Hobbs, R. W. (2011). A framework for 3-D joint inversion of MT, gravity and seismic refraction data. *Geophysical Journal International*, 184(1):477–493.
- Morgan, J. and Rebolledo-Vieyra, M. (2013). Geophysical studies of impact craters. *Impact Cratering: Processes and Products*, pages 211–222.
- Morgan, J., Warner, M., Arnoux, G., Hooft, E., Toomey, D., VanderBeek, B., and Wilcock, W. (2016). Next-generation seismic experiments–II: wide-angle, multi-azimuth, 3-D, full-waveform inversion of sparse field data. *Geophysical Journal International*, 204(2):1342–1363.
- Morgan, J., Warner, M., Bell, R., Ashley, J., Barnes, D., Little, R., Roele, K., and Jones, C. (2013). Next-generation seismic experiments: wide-angle, multi-azimuth, three-dimensional, full-waveform inversion. *Geophysical Journal International*, 195(3):1657–1678.
- Moser, T. (1991). Shortest path calculation of seismic rays. *Geophysics*, 56(1):59–67.
- Moser, T., Nolet, G., and Snieder, R. (1992). Ray bending revisited. *Bulletin of the Seismological Society of America*, 82(1):259–288.
- Müntener, O., Kelemen, P., and Grove, T. (2001). The role of H₂O and composition on the genesis of igneous pyroxenites: An experimental study. *Contrib. Mineral. Petrol*, 141:643–658.
- Murphy, M., Sparks, R., Barclay, J., Carroll, M., and Brewer, T. (2000). Remobilization of andesite magma by intrusion of mafic magma at the Soufrière Hills Volcano, Montserrat, West Indies. *Journal of petrology*, 41(1):21–42.
- Norris, A. (1989). An examination of the Mori-Tanaka effective medium approximation for multiphase composites. *Journal of Applied Mechanics*, 56(1):83–88.
- O’Connell, R. J. and Budiansky, B. (1977). Viscoelastic properties of fluid-saturated cracked solids. *Journal of Geophysical Research*, 82(36):5719–5735.

- Oldham, R. D. (1906). The constitution of the interior of the Earth, as revealed by earthquakes. *Quarterly Journal of the Geological Society*, 62(1-4):456–475.
- Operto, S., Gholami, Y., Prioux, V., Ribodetti, A., Brossier, R., Metivier, L., and Virieux, J. (2013). A guided tour of multiparameter full-waveform inversion with multicomponent data: From theory to practice. *The Leading Edge*.
- Paterson, S. R., Fowler, T. K., and Miller, R. B. (1996). Pluton emplacement in arcs: a crustal-scale exchange process. *Geological Society of America Special Papers*, 315:115–123.
- Paterson, S. R., Okaya, D., Memeti, V., Economos, R., and Miller, R. B. (2011). Magma addition and flux calculations of incrementally constructed magma chambers in continental margin arcs: Combined field, geochronologic, and thermal modeling studies. *Geosphere*, 7(6):1439–1468.
- Paulatto, M., Annen, C., Henstock, T. J., Kiddle, E., Minshull, T. A., Sparks, R., and Voight, B. (2012). Magma chamber properties from integrated seismic tomography and thermal modeling at Montserrat. *Geochemistry, Geophysics, Geosystems*, 13(1).
- Paulatto, M., Minshull, T., Baptie, B., Dean, S., Hammond, J., Henstock, T., Kenedi, C., Kiddle, E., Malin, P., Peirce, C., et al. (2010). Upper crustal structure of an active volcano from refraction/reflection tomography, Montserrat, Lesser Antilles. *Geophysical Journal International*, 180(2):685–696.
- Petford, N. (1996). Dykes or diapirs? *Earth and Environmental Science Transactions of the Royal Society of Edinburgh*, 87(1-2):105–114.
- Petford, N., Atherton, M., and Halliday, A. (1996). Rapid magma production rates, underplating and remelting in the Andes: Isotopic evidence from northern-central Peru (9–11 S). *Journal of South American Earth Sciences*, 9(1):69–78.
- Petford, N., Cruden, A., McCaffrey, K., and Vigneresse, J.-L. (2000). Granite magma formation, transport and emplacement in the Earth’s crust. *Nature*, 408(6813):669–673.
- Petford, N. and Gallagher, K. (2001). Partial melting of mafic (amphibolitic) lower crust by periodic influx of basaltic magma. *Earth and Planetary Science Letters*, 193(3):483–499.
- Petford, N. and Koenders, M. (1998). Self-organisation and fracture connectivity in rapidly heated continental crust. *Journal of Structural Geology*, 20:1425–1434.
- Plessix, R.-E. (2008). Introduction: Towards a full waveform inversion. *Geophysical Prospecting*, 56(6):761–763.

- Plessix, R.-E. and Perkins, C. (2010). Thematic Set: Full waveform inversion of a deep water ocean bottom seismometer dataset. *First Break*, 28(4):71–78.
- Pratt, R., Song, Z.-M., Williamson, P., and Warner, M. (1996). Two-dimensional velocity models from wide-angle seismic data by wavefield inversion. *Geophysical Journal International*, 124(2):323–340.
- Pratt, R. G. (1999). Seismic waveform inversion in the frequency domain, Part 1: Theory and verification in a physical scale model. *Geophysics*, 64(3):888–901.
- Prieux, V., Brossier, R., Operto, S., and Virieux, J. (2013a). Multiparameter full waveform inversion of multicomponent ocean-bottom-cable data from the Valhall field. Part 1: Imaging compressional wave speed, density and attenuation. *Geophysical Journal International*, 194(3):1640–1664.
- Prieux, V., Brossier, R., Operto, S., and Virieux, J. (2013b). Multiparameter full waveform inversion of multicomponent ocean-bottom-cable data from the Valhall field. Part 2: Imaging compressive-wave and shear-wave velocities. *Geophysical Journal International*, 194(3):1665–1681.
- Quick, J. E., Sinigoi, S., and Mayer, A. (1994). Emplacement dynamics of a large mafic intrusion in the lower crust, Ivrea-Verbano Zone, northern Italy. *Journal of Geophysical Research: Solid Earth*, 99(B11):21559–21573.
- Quick, J. E., Sinigoi, S., Negrini, L., Demarchi, G., and Mayer, A. (1992). Synmagmatic deformation in the underplated igneous complex of the Ivrea-Verbano zone. *Geology*, 20(7):613–616.
- Ranalli, G. (1987). Rheology of the Earth: Deformation and Flow Processes in Geophysics and Geodynamics, 366 pp.
- Ratcliffe, A., Win, C., Vinje, V., Conroy, G., Warner, M., Umpleby, A., Stekl, I., Nangoo, T., Bertrand, A., et al. (2011). Full waveform inversion: A North Sea OBC case study. In *2011 SEG Annual Meeting*. Society of Exploration Geophysicists.
- Rawlinson, N. and Sambridge, M. (2003). Seismic travelttime tomography of the crust and lithosphere. *Advances in Geophysics*, 46:81–199.
- Rea, W. J. (1974). The volcanic geology and petrology of Montserrat, West Indies. *Journal of the Geological Society*, 130(4):341–366.
- Reuss, A. (1929). Berechnung der fließgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 9(1):49–58.

- Richter, F. M. and McKenzie, D. (1984). Dynamical models for melt segregation from a deformable matrix. *The Journal of Geology*, 92(6):729–740.
- Riel, N., Bouilhol, P., Magni, V., van Hunen, J., and Velic, M. (2016). Coupled thermodynamic and two-phase flow modelling of partially melting crust. *EGU General Assembly Conference Abstracts*, 18:17443.
- Riel, N., Bouilhol, P., van Hunen, J., Cornet, J., Magni, V., Grigorova, V., and Velic, M. (2018). Interaction between mantle-derived magma and lower arc crust: quantitative reactive melt flow modelling using STyx. *Geological Society, London, Special Publications*, 478:SP478–6.
- Rivers, M. L. and Carmichael, I. S. (1987). Ultrasonic studies of silicate melts. *Journal of Geophysical Research: Solid Earth*, 92(B9):9247–9270.
- Roobol, M. and Smith, A. (1998). Pyroclastic stratigraphy of the Soufrière Hills Volcano, Montserrat—Implications for the present eruption. *Geophysical Research Letters*, 25(18):3393–3396.
- Rosenberg, C. and Handy, M. (2005). Experimental deformation of partially melted granite revisited: implications for the continental crust. *Journal of metamorphic Geology*, 23(1):19–28.
- Rushmer, T. (1991). Partial melting of two amphibolites: contrasting experimental results under fluid-absent conditions. *Contributions to Mineralogy and Petrology*, 107(1):41–59.
- Rutherford, M. J. and Hill, P. M. (1993). Magma ascent rates from amphibole breakdown: an experimental study applied to the 1980–1986 Mount St. Helens eruptions. *Journal of Geophysical Research*, 98(19):667–685.
- Rypina, I. I. and Brown, M. G. (2007). On the width of a ray. *The Journal of the Acoustical Society of America*, 122(3):1440–1448.
- Sawyer, E. (1994). Melt segregation in the continental crust. *Geology*, 22(11):1019–1022.
- Sawyer, E. (1996). Melt segregation and magma flow in migmatites: implications for the generation of granite magmas. *Geological Society of America Special Papers*, 315:85–94.
- Scarpa, R. (2001). Predicting volcanic eruptions. *Science*, 293(5530):615–616.
- Schmeling, H. (1985). Numerical models on the influence of partial melt on elastic, anelastic and electric properties of rocks. Part I: elasticity and anelasticity. *Physics of the earth and planetary interiors*, 41(1):34–57.

- Schoene, B., Schaltegger, U., Brack, P., Latkoczy, C., Stracke, A., and Günther, D. (2012). Rates of magma differentiation and emplacement in a ballooning pluton recorded by U–Pb TIMS-TEA, Adamello batholith, Italy. *Earth and Planetary Science Letters*, 355:162–173.
- Shalev, E., Kenedi, C., Malin, P., Voight, V., Miller, V., Hidayat, D., Sparks, R., Minshull, T., Paulatto, M., Brown, L., et al. (2010). Three-dimensional seismic velocity tomography of Montserrat from the SEA-CALIPSO offshore/onshore experiment. *Geophysical Research Letters*, 37(19).
- Shepherd, J., Tomblin, J., and Woo, D. (1971). Volcano-seismic crisis in Montserrat, West Indies, 1966–67. *Bulletin volcanologique*, 35(1):143–162.
- Shillington, D. J., Van Avendonk, H. J., Holbrook, W. S., Kelemen, P. B., and Hornbach, M. J. (2004). Composition and structure of the central Aleutian island arc from arc-parallel wide-angle seismic data. *Geochemistry, Geophysics, Geosystems*, 5(10).
- Sigurdsson, H., Cashdollar, S., and Sparks, S. R. (1982). The eruption of Vesuvius in AD 79: reconstruction from historical and volcanological evidence. *American journal of archaeology*, pages 39–51.
- Simmons, G. and Wang, H. (1971). Single crystal elastic constants and calculated aggregate properties. In *Mass., MIT Press*.
- Sinigoi, S., Quick, J. E., Clemens-Knott, D., Mayer, A., Demarchi, G., Mazzucchelli, M., Negrini, L., and Rivalenti, G. (1994). Chemical evolution of a large mafic intrusion in the lower crust, Ivrea-Verbano Zone, northern Italy. *Journal of Geophysical Research: Solid Earth*, 99(B11):21575–21590.
- Sirgue, L. (2006). The importance of low frequency and large offset in waveform inversion. In *68th EAGE Conference and Exhibition incorporating SPE EUROPEC 2006*.
- Sirgue, L., Barkved, O., Dellinger, J., Etgen, J., Albertin, U., and Kommedal, J. (2010a). Thematic set: Full waveform inversion: The next leap forward in imaging at Valhall. *First Break*, 28(4):65–70.
- Sirgue, L., Etgen, J., and Albertin, U. (2007). 3D full-waveform inversion: Wide-versus narrow-azimuth acquisitions. In *SEG Technical Program Expanded Abstracts 2007*, pages 1760–1764. Society of Exploration Geophysicists.
- Sirgue, L., Etgen, J. T., Albertin, U., and Brandsberg-Dahl, S. (2010b). System and method for 3D frequency domain waveform inversion based on 3D time-domain forward modeling. US Patent 7,725,266.

- Sisson, T., Ratajeski, K., Hankins, W., and Glazner, A. F. (2005). Voluminous granitic magmas from common basaltic sources. *Contributions to Mineralogy and Petrology*, 148(6):635–661.
- Sleep, N. H. (1974). Segregation of magma from a mostly crystalline mush. *GSA Bulletin*, 85(8):1225–1232.
- Smith, C. S. (1964). Some elementary principles of polycrystalline microstructure. *Metallurgical Reviews*, 9(1):1–48.
- Smith, T. M., Sondergeld, C. H., and Rai, C. S. (2003). Gassmann fluid substitutions: A tutorial. *Geophysics*, 68(2):430–440.
- Solano, J. (2011). *Numerical Modelling of Melt Intrusion Within and Around Sill Intrusions*. PhD Thesis, Imperial College London.
- Solano, J., Jackson, M., Sparks, R., and Blundy, J. (2014). Evolution of major and trace element composition during melt migration through crystalline mush: implications for chemical differentiation in the crust. *American Journal of Science*, 314(5):895–939.
- Solano, J., Jackson, M., Sparks, R., Blundy, J., and Annen, C. (2012). Melt segregation in deep crustal hot zones: a mechanism for chemical differentiation, crustal assimilation and the formation of evolved magmas. *Journal of Petrology*, 53(10):1999–2026.
- Sparks, R. (2003). Forecasting volcanic eruptions. *Earth and Planetary Science Letters*, 210(1):1–15.
- Spera, F. J. and Bohron, W. A. (2004). Open-system magma chamber evolution: An energy-constrained geochemical model incorporating the effects of concurrent eruption, recharge, variable assimilation and fractional crystallization (EC-E? RA χ FC). *Journal of Petrology*, 45(12):2459–2480.
- Spitzer, R., White, R. S., et al. (2005). Advances in seismic imaging through basalts: a case study from the Faroe Shetland Basin. *Petroleum Geoscience*, 11(2):147–156.
- Stacey, F. and Isaak, D. (2003). Anharmonicity in mineral physics: a physical interpretation. *Journal of Geophysical Research: Solid Earth*, 108(B9).
- Staples, R. K., White, R. S., Brandsdóttir, B., Menke, W., Maguire, P. K., and McBride, J. H. (1997). Faeroe-Iceland Ridge Experiment 1. Crustal structure of northeastern Iceland. *Journal of Geophysical Research: Solid Earth*, 102(B4):7849–7866.
- Sun, Z., Li, S., Ahuja, R., and Schneider, J. M. (2004). Calculated elastic properties of M₂AlC (M= Ti, V, Cr, Nb and Ta). *Solid state communications*, 129(9):589–592.

- Takahashi, N., Kodaira, S., Klemperer, S. L., Tatsumi, Y., Kaneda, Y., and Suyehiro, K. (2007). Crustal structure and evolution of the Mariana intra-oceanic island arc. *Geology*, 35(3):203–206.
- Tarantola, A. (1984). Inversion of seismic reflection data in the acoustic approximation. *Geophysics*, 49(8):1259–1266.
- Tarantola, A. (1987). Inverse problem theory. *Elsevier*.
- Te Wu, T. (1966). The effect of inclusion shape on the elastic moduli of a two-phase material. *International Journal of solids and structures*, 2(1):1–8.
- Tepper, J. H., Nelson, B. K., Bergantz, G. W., and Irving, A. J. (1993). Petrology of the Chilliwack batholith, North Cascades, Washington: generation of calc-alkaline granitoids by melting of mafic lower crust with variable water fugacity. *Contributions to Mineralogy and Petrology*, 113(3):333–351.
- Toomey, D. R., Solomon, S. C., and Purdy, G. (1994). Tomographic imaging of the shallow crustal structure of the East Pacific Rise at 9° 30' N. *Journal of Geophysical Research: Solid Earth*, 99(B12):24135–24157.
- Trofimovs, J., Talling, P., Fisher, J., Sparks, R., Watt, S., Hart, M., Smart, C., Le Friant, A., Cassidy, M., Moreton, S., et al. (2013). Timing, origin and emplacement dynamics of mass flows offshore of SE Montserrat in the last 110 ka: Implications for landslide and tsunami hazards, eruption history, and volcanic island evolution. *Geochemistry, Geophysics, Geosystems*, 14(2):385–406.
- Van Avendonk, H. J., Harding, A. J., Orcutt, J. A., and McClain, J. S. (1998). A two-dimensional tomographic study of the Clipperton transform fault. *Journal of Geophysical Research: Solid Earth*, 103(B8):17885–17899.
- Van Avendonk, H. J. A. (1998). *An investigation of the crustal structure of the Clipperton transform fault area using 3D seismic tomography*. PhD thesis, University of California, San Diego.
- Vidale, J. (1988). Finite-difference calculation of travel times. *Bulletin of the Seismological Society of America*, 78(6):2062–2076.
- Vigh, D., Kapoor, J., and Li, H. (2011). Full-waveform inversion application in different geological settings. In *SEG Technical Program Expanded Abstracts 2011*, pages 2374–2378. Society of Exploration Geophysicists.
- Vigh, D., Kapoor, J., and Moldoveanu, N. (2013). Long offset aided full waveform inversion. In *13th International Congress of the Brazilian Geophysical Society & EXPOGEF, Rio de Janeiro, Brazil*,

- 26–29 August 2013, pages 294–297. Society of Exploration Geophysicists and Brazilian Geophysical Society.
- Vignerresse, J. and Clemens, J. (2000). Granitic magma ascent and emplacement: neither diapirism nor neutral buoyancy. *Geological Society, London, Special Publications*, 174(1):1–19.
- Vignerresse, J. L. (1995). Control of granite emplacement by regional deformation. *Tectonophysics*, 249(3):173–186.
- Villasenor, A., Benz, H., and Power, J. (1996). Three-dimensional P-wave velocity model for Soufrière Hills Volcano, Montserrat, W.I. *The Soufrière Hills Eruption, Montserrat*.
- Virieux, J. and Operto, S. (2009). An overview of full-waveform inversion in exploration geophysics. *Geophysics*, 74(6):WCC1–WCC26.
- Voight, B. and Sparks, R. (2010). Introduction to special section on the Eruption of Soufrière Hills Volcano, Montserrat, the CALIPSO Project, and the SEA-CALIPSO Arc-Crust Imaging Experiment. *Geophysical Research Letters*, 37(19).
- Voight, B., Sparks, R., Shalev, E., Minshull, T., Paulatto, M., Annen, C., Kenedi, C., Hammond, J., Henstock, T., Brown, L., et al. (2014). The SEA-CALIPSO volcano imaging experiment at Montserrat: plans, campaigns at sea and on land, scientific results, and lessons learned. *Geological Society, London, Memoirs*, 39(1):253–289.
- Voight, B., Widiwijayanti, C., Mattioli, G., Elsworth, D., Hidayat, D., and Strutt, M. (2010). Magma-sponge hypothesis and stratovolcanoes: Case for a compressible reservoir and quasi-steady deep influx at Soufrière Hills Volcano, Montserrat. *Geophysical Research Letters*, 37(19).
- Voigt, W. (1928). Textbook of crystal physics. *BB Teubner, Leipzig*, 2.
- Wadge, G., Mattioli, G., and Herd, R. (2006). Ground deformation at Soufrière Hills Volcano, Montserrat during 1998–2000 measured by radar interferometry and GPS. *Journal of Volcanology and Geothermal Research*, 152(1-2):157–173.
- Wadge, G., Scheuchl, B., Cabey, L., Palmer, M., Riley, C., Smith, A., and Stevens, N. (1999). Operational use of InSAR for volcano observatories: experience from Montserrat. In *Proc. FRINGE99 symposium*, page 8. Citeseer.
- Waff, H. and Bulau, J. R. (1979). Equilibrium fluid distribution in an ultramafic partial melt under hydrostatic stress conditions. *Journal of Geophysical Research: Solid Earth*, 84(B11):6109–6114.

- Walsh, J. (1969). New analysis of attenuation in partially melted rock. *Journal of Geophysical Research*, 74(17):4333–4337.
- Ward, K. M., Zandt, G., Beck, S. L., Christensen, D. H., and McFarlin, H. (2014). Seismic imaging of the magmatic underpinnings beneath the Altiplano-Puna volcanic complex from the joint inversion of surface wave dispersion and receiver functions. *Earth and Planetary Science Letters*, 404:43–53.
- Wark, D. A. and Watson, E. B. (1998). Grain-scale permeabilities of texturally equilibrated, monomineralic rocks. *Earth and Planetary Science Letters*, 164(3):591–605.
- Warner, M., Ratcliffe, A., Nangoo, T., Morgan, J., Umpleby, A., Shah, N., Vinje, V., Štekl, I., Guasch, L., Win, C., et al. (2013). Anisotropic 3D full-waveform inversion. *Geophysics*, 78(2):R59–R80.
- Watt, J. P. (1980). Hashin-Shtrikman bounds on the effective elastic moduli of polycrystals with monoclinic symmetry. *Journal of Applied Physics*, 51(3):1520–1524.
- Watt, J. P., Davies, G. F., and O’Connell, R. J. (1976). The elastic properties of composite materials. *Reviews of Geophysics*, 14(4):541–563.
- Watt, J. P. and Peselnick, L. (1980). Clarification of the Hashin-Shtrikman bounds on the effective elastic moduli of polycrystals with hexagonal, trigonal, and tetragonal symmetries. *Journal of Applied Physics*, 51(3):1525–1531.
- Weill, D., Stebbins, J., Hon, R., and Carmichael, I. (1980). The enthalpy of fusion of anorthite. *Contributions to Mineralogy and Petrology*, 74(1):95–102.
- Weinberg, R. F. (1996). Ascent mechanism of felsic magmas: news and views. *Geological Society of America Special Papers*, 315:95–103.
- White, D. and Bolland, A. (1992). A comparison of forward modeling and inversion of seismic first arrivals over the Kapuskasing Uplift. *Bulletin of the Seismological Society of America*, 82(1):304–322.
- White, R. S., Smallwood, J. R., Flidner, M. M., Boslaugh, B., Maresh, J., and Fruehn, J. (2003). Imaging and regional distribution of basalt flows in the Faeroe-Shetland Basin. *Geophysical Prospecting*, 51(3):215–231.
- White, R. S., Spitzer, R., Christie, P., Roberts, A., Lunnon, Z., Maresh, J., iSimm Working Group, et al. (2005). Seismic imaging through basalt flows on the Faroes Shelf. In *Proceedings of the 1st Faroe Islands Exploration Conference: Annal. Soc. Scient. Færoensis, Supplementum*, volume 43, pages 11–31.

- Wickham, S. (1987). The segregation and emplacement of granitic magmas. *Journal of the Geological Society*, 144(2):281–297.
- Williamson, P. (1991). A guide to the limits of resolution imposed by scattering in ray tomography. *Geophysics*, 56(2):202–207.
- Williamson, P. R. and Worthington, M. (1993). Resolution limits in ray tomography due to wave behavior: Numerical experiments. *Geophysics*, 58(5):727–735.
- Wilson, C., Blake, S., Charlier, B., and Sutton, A. (2005). The 26· 5 ka Oruanui eruption, Taupo volcano, New Zealand: development, characteristics and evacuation of a large rhyolitic magma body. *Journal of Petrology*, 47(1):35–69.
- Wolf, M. and Wyllie, P. (1991). Dehydration-melting of solid amphibolite at 10 kbar: textural development, liquid interconnectivity and applications to the segregation of magmas. *Mineralogy and Petrology*, 44(3):151–179.
- Woodward, M. J., Nichols, D., Zdraveva, O., Whitfield, P., and Johns, T. (2008). A decade of tomography. *Geophysics*, 73(5):VE5–VE11.
- Wotzlaw, J.-F., Bindeman, I. N., Watts, K. E., Schmitt, A. K., Caricchi, L., and Schaltegger, U. (2014). Linking rapid magma reservoir assembly and eruption trigger mechanisms at evolved Yellowstone-type supervolcanoes. *Geology*, 42(9):807–810.
- Yoshinobu, A. S., Okaya, D. A., and Paterson, S. R. (1998). Modeling the thermal evolution of fault-controlled magma emplacement models: implications for the solidification of granitoid plutons. *Journal of Structural Geology*, 20(9):1205–1218.
- Young, S. R., Sparks, R. S. J., Aspinall, W. P., Lynch, L. L., Miller, A. D., Robertson, R. E., and Shepherd, J. B. (1998). Overview of the eruption of Soufrière Hills volcano, Montserrat, 18 July 1995 to December 1997. *Geophysical Research Letters*, 25(18):3389–3392.
- Zellmer, G., Hawkesworth, C., Sparks, R., Thomas, L., Harford, C., Brewer, T., and Loughlin, S. (2003a). Geochemical evolution of the Soufrière Hills volcano, Montserrat, Lesser Antilles volcanic arc. *Journal of Petrology*, 44(8):1349–1374.
- Zellmer, G., Sparks, R., Hawkesworth, C., and Wiedenbeck, M. (2003b). Magma emplacement and remobilization timescales beneath Montserrat: insights from Sr and Ba zonation in plagioclase phenocrysts. *Journal of Petrology*, 44(8):1413–1431.

- Zelt, C. A. (1998). Lateral velocity resolution from three-dimensional seismic refraction data. *Geophysical Journal International*, 135(3):1101–1112.
- Zelt, C. A. (1999). Modelling strategies and model assessment for wide-angle seismic traveltimes data. *Geophysical Journal International*, 139(1):183–204.
- Zelt, C. A., Sain, K., Naumenko, J. V., and Sawyer, D. S. (2003). Assessment of crustal velocity models using seismic refraction and reflection tomography. *Geophysical Journal International*, 153(3):609–626.
- Zhang, J. and Toksöz, M. N. (1998). Nonlinear refraction traveltimes tomography. *Geophysics*, 63(5):1726–1737.
- Ziolkowski, A., Hanssen, P., Gatliff, R., Jakubowicz, H., Dobson, A., Hampson, G., Li, X.-Y., and Liu, E. (2003). Use of low frequencies for sub-basalt imaging. *Geophysical Prospecting*, 51(3):169–182.