École Normale Supérieure de Lyon
Laboratoire de Sciences de la Terre

Charles University in Prague
Faculty of Mathematics and Physics

Summary of Doctoral Thesis

Modeling of two-phase flow in geophysics: partial melting, compaction and differentiation

Ondřej Šrámek

Supervisors: Yanick Ricard & Ondřej Čadek

Department of Geophysics
V Holešovičkách 2
180 00 Praha 8
Czech Republic

Prague, 2007

École Normale Supérieure de Lyon
Laboratoire de Sciences de la Terre

Université Charles à Prague
Faculté de mathématiques et physique

Résumé de la thèse de doctorat

Modèle d'écoulement biphasé en sciences de la Terre : fusion partielle, compaction et différenciation

Ondřej Šrámek

Directeurs de thèse : Yanick Ricard & Ondřej Čadek

Department of Geophysics
V Holešovičkách 2
180 00 Praha 8
Czech Republic

Prague, 2007

École Normale Supérieure de Lyon
Laboratoire de Sciences de la Terre

Univerzita Karlova v Praze
Matematicko-fyzikální fakulta

Autoreferát dizertační práce

Modelování prostředí o dvou fázích v geofyzice: částečné tání, kompakce a diferenciace

Ondřej Šrámek

Školitetelé: Yanick Ricard & Ondřej Čadek

Katedra geofyziky
V Holešovičkách 2
180 00 Praha 8

Praha, 2007

Dizertace byla vypracována na základě výsledků získaných v letech 2002–2007 během doktorandského studia v Laboratoire de Sciences de la Terre, École Normale Supérieure de Lyon ve Francii a na Katedře geofyziky MFF UK v Praze.

Dizertant:
Ondřej Šrámek
Laboratoire de Sciences de la Terre, UMR 5570, CNRS, Université de Lyon
ENS Lyon, 46 allée d'Italie, 69364 Lyon cédex 07, France
&
Katedra geofyziky MFF UK
V Holešovičkách 2, 180 00 Praha 8
`sramek@geo.mff.cuni.cz`
`http://geo.mff.cuni.cz/~sramek/`

Obor studia:
F-7: Geofyzika

Školitelé:
Yanick Ricard
Laboratoire de Sciences de la Terre, UMR 5570, CNRS, Université de Lyon
UCB Lyon 1, 2 rue Raphaël Dubois, 69622 Villeurbanne cédex, France

Ondřej Čadek
Katedra geofyziky MFF UK
V Holešovičkách 2, 180 00 Praha 8

Oponenti:
Neil Ribe
Dynamique des Fluides Géologiques, Institut de Physique du Globe
4 place Jussieu, 75252 Paris cédex 05, France

Harro Schmeling
Faculty of Earth Sciences, Section Geophysics, J. W. Goethe University
Altenhöferallee 1, 60438 Frankfurt M, Germany

Předseda oborové rady:
Oldřich Novotný
Katedra geofyziky MFF UK
V Holešovičkách 2, 180 00 Praha 8

Obhajoba dizertace se koná dne 20.12.2007 ve 14 hodin v posluchárně L na École Normale Supérieure de Lyon, 46 allée d'Italie, Lyon, Francie.

Contents

1 Abstract

Partial melting and migration of melts play an important role in the formation and evolution of the Earth. Transport of heat, rock rheology and distribution of major, minor, as well volatile chemical species are all affected by the presence and migration of magmas. Partial melting and melt extraction are central processes for the formation of the oceanic crust and are responsible for the depletion in incompatible elements of the mantle part of the lithosphere. Migration of molten material played a major role in the dynamical evolution of the early Earth and even now plays a fundamental role in the transport of matter as well as heat in partially molten regions of deeper mantle (e.g, at the core–mantle boundary).

The separation of the denser metal from the lighter silicates is the most extensive differentiation process in the course of Earth's evolution – and the evolution of terrestrial planetary bodies in general. This process also implies the presence of distinct phases, in solid and liquid states. Gravitational energy which is released upon differentiation is a major source of heat that must be considered when assessing the thermal history of a forming planet. It is therefore essential to properly take into account the energy exchange that takes place in a multiphase medium on a large spatial scale in order to investigate early planetary evolution and to constrain the differentiation time scales.

Theoretical analyses and numerical modeling are essential tools for the study of the planetary dynamics at global scale. We present a new general model of two-phase flow and deformation in a two-phase medium. Our model is a modification of a recent set of equations presented by Bercovici *et al.* (2001a), extended so that it allows for the mass exchange between phases (that is, phase change – melting/solidification). The model offers a self-consistent description of the mechanics and thermodynamics of a mixture of two viscous fluids in the form of continuum mechanical equations, in the limit of a slow creeping flow. The difference in pressures that exists between the two phases is generated i) by the surface tension at the interfaces between the phases which are included in the description, and ii) by the isotropic deformation (i.e., compaction or dilation) of the individual phases upon flow.

In all the geologic applications considered, one of the phases (named the 'liquid' phase) is much less viscous than the other phase (the 'solid' phase), which largely simplifies the equations. In the modeling of differentiation of a terrestrial planet, the 'solid' phase represents the silicates of the mantle and the 'liquid' phase is the iron alloy of the core. Depending on the temperature, the iron phase can itself be either molten or in its solid state. There is no mass transfer between the silicate and the iron phase. First we study the compaction in a layer and of a spherically symmetric body (1-D models). A numerical code and various simulation in 2-D are then presented. For a protoplanet of a radius of $\sim 2000\,\mathrm{km}$, we obtain characteristic time scales of the core segregation of the order of $0.1\,\mathrm{Myr}$.

The careful treatment of the phase change in the two-phase model, based of the fundamental principles of thermodynamics in a non-equilibrium case, allows us to study the coupling between the viscous deformation and melting. We present an analysis of the pressure release melting of an upwelling mantle below a spreading center. The volumetric deformation of the matrix skeleton generates a dynamic pressure difference between the solid and the melt: the magma is submitted to a lower pressure than the compacting

solid matrix. This effect is particularly important at incipient melting and can move the base of the melting zone by few km. The effect of the surface tension on the initiation of melting is also discussed; it depends on the energetic balance of the solid–solid and solid–melt interfaces on the grain scale, and consequently on the geometry of the first melt to appear. The magma extraction velocities reach at most ten times the upwelling velocity of the solid. The porosity (melt volume fraction) remains small (few percent) even at high degree of meting, and has a roughly parabolic profile in the entire melting zone.

2 Introduction

Two-phase flow is a phenomenon of capital importance in the Earth's interior. The two main contexts involving two-phase dynamics that we discuss are partially molten regions of the mantle and the process of differentiation of the Earth's metallic core from the silicate mantle.

The most extensive magma production in the Earth's interior is related to accretion of tectonic plates at mid ocean ridges. The space between the spreading plates is continuously being filled with material ascending from deeper parts of the mantle. The pressure release upon this roughly adiabatic ascent causes the temperature to increase above the solidus of the mantle rock and partial melting occurs. The lighter magma moves through the solid towards the surface where is resolidifies, thus creating a new oceanic crust. The solid residue after melting forms the mantle part of the lithosphere. Other major settings of near surface melting include island arcs and volcanic arcs at subduction zones, and melting at hot spots. Presence of partially molten regions deeper in the Earth's mantle has also been proposed (for example, at the top of the transition zone or at the bottom of the mantle). Melting and partially molten zones involve the presence of two distinct phases, both of which move – each phase at its own velocity – and deform and where mass is transfered from one phase to the other upon melting and freezing.

The Earth has a dense metallic core overlain by a lighter silicate mantle. Such first order layering is also inferred for other terrestrial bodies in the Solar System. This structure is readily explained in terms of minimization of gravitational potential energy but it is not clear by what mechanism and on what time scales the differentiation occurred; the building material of a terrestrial planet in the solar nebula is thought to have had homogeneous distribution of metal and silicates. Geochemical arguments suggest that the differentiation was contemporaneous or only happened shortly after the planetary accretion process. The separation of metal from the silicates probably involved several mechanisms, depending on the actual size of the growing planet, its thermal state and the depth within the planet. It also implied the presence of two (or more) phases – potentially both silicates and metal in their solid and liquid state. Geodynamical modeling of these two-phase (multi-phase) phenomena gives us insight into the dynamics and evolution of a young Earth.

3 Two-phase model

Both of the two processes discussed above involve flow and deformation of a two-phase medium. An appropriate theoretical model is needed in order to investigate the evolution and the dynamics of the deforming two-phase medium. The approach we take is one based on the *classical averaging theory* (e.g., Drew & Passman, 1998). The actual distribution of the two phases as well as various physical quantities are averaged over a "control volume" on a mesoscopic scale. It is assumed that the two phases are present everywhere with continuously varying concentrations. A set of coupled equations is written in the two-phase region. This approach is justified by the fact that in geophysics, the typical size of the region of study is much larger than the characteristic grain/pore size in the two-phase mixture. An alternative approach would be to solve a separate set of equations in each single-phase domain and match appropriate quantities along the interface between the phases; this is the preferred method if one studies the evolution of a small number of large isolated blobs and requires an often cumbersome tracking of the interfacial surface.

We seek a set of continuum mechanical equations that express the basic conservation laws – of mass, momentum and energy, combined with the constitutive equations and other necessary phenomenological relations. The first geophysical models of two-phase flow appeared in the 1970's (Sleep, 1974; Turcotte & Ahern, 1978; Ahern & Turcotte, 1979). McKenzie (1984) formulated a general model of a partially molten rock which has been widely used in modeling of partially molten zones and magma migration. The mechanical interaction between the solid rock and the magma corresponds to percolation of a viscous liquid through a porous solid matrix – that is, a "Darcy-type" flow (Darcy, 1856). In addition, the solid itself is a viscous fluid (with much higher viscosity than the magma) and deforms.

In a recent series of articles, Bercovici *et al.* (2001a,b) and Ricard *et al.* (2001) revisited the two-phase modeling problematics and presented a model that is more general than McKenzie's equations in several aspects:

1. The ratio of viscosities of the two phases is arbitrary; one of the phases is not necessarily much less viscous than the other. In fact this free choice of viscosity values makes the set of equations invariant to the permutation of phases which is exploited in the model development.

2. The presence of the interface between the phases is accounted for. The interface has its surface energy and the two-phase mixture is acted upon by an interfacial surface force.

3. One of the principal motivations for this new model was to create a formalism that also includes "damage". Damage is generated by the deposition of energy on the interface. It is manifested as the creation, growth and propagation of micro-cracks and cavities (Bercovici *et al.*, 2001a,b; Bercovici & Ricard, 2003) and the change in grain size (Bercovici & Ricard, 2005). Damage is one possible mechanism for focusing the deformation in the lithosphere, therefore it offers a possible model for the generation of tectonic plates.

The equations proposed by McKenzie (1984) permit phase change from solid to liquid and vice versa (melting/freezing). However the rate of phase change is not predicted by the model and has to be prescribed; the flow and the phase change are effectively decoupled in McKenzie's equations. But the deformation of the two-phase mixture upon melt extraction creates local pressure perturbations and in consequence the melting rate, which is necessarily pressure- and temperature-dependent, will be modified. A non-uniform melting rate can then lead to heterogeneity in magma distribution and may give rise to porosity instabilities.

We extend the new model of Bercovici *et al.* (2001a) so that it is applicable to problems of partial melting and magma extraction. We introduce the phase change in the equations and obtain a relation for the melting rate in a self-consistent way using the principles of non-equilibrium thermodynamics. We thus obtain a general model that includes the coupling between phase change, two-phase flow, viscous deformation and interfacial effects. In the following paragraphs we summarize the common points and the differences between the McKenzie's model (McKenzie, 1984) and our new model (Šrámek *et al.*, 2007).

Common points of McKenzie (1984) and our new model

- Both models describe the two-phase flow by continuum mechanical partial differential equations for quantities that are averaged on a mesoscopic scale (that is, over a domain that contains a large number of grains/pores but that is much smaller than the region of interest).
- Inertia and kinetic energy are neglected. In this creeping flow approximation the acceleration is zero and forces are always in balance.
- Isotropy of the spatial distribution and orientation of pores/grains is assumed.
- The two phases are viscous liquids; elastic deformation is not considered.
- In the case of a rigid matrix, the flow of the low viscosity liquid is a classical Darcy percolation.

Differences between McKenzie (1984) and our new model

- In terms of rheology, in McKenzie (1984) the solid matrix is a compressible fluid and its rheological relation contains two viscosities (bulk viscosity and shear viscosity), and the liquid phase is an incompressible fluid with negligible viscosity. In our model both phases are viscous fluids of arbitrary viscosities, individually incompressible. The geophysical limit of a large viscosity difference is made *a posteriori.*
- McKenzie (1984) neglects surface tension. In our model the surface tension and interfacial effects are considered. In particular the surface tension affects the phase change (i.e., the Gibbs-Thomson effect). The extension of our model so that it includes damage (that is, in the lines of Bercovici *et al.*, 2001a) is possible but not done here.
- The consideration of interfaces and surface tension implies the difference in pressure between the phases. Moreover, this pressure difference has a static contribution due to surface forces on a curved interface as well as a dynamical contribution related to compaction or dilation of the skeleton of each phase. The pressure difference is therefore non-zero even if surface tension is negligible as long as the two-phase medium is deforming.

- The melting rate (or an equivalent quantity that describes the mass transfer between phases) is an external (prescribed) quantity in McKenzie (1984). In our model the proper coupling between the equation for the melting rate and the flow equations permits us to study the effect of the dynamical deformation on the phase change. On the other hand, unlike McKenzie, we limit our study to a univariant phase change.

New two-phase model with phase change coupled to deformation

Here we present the equations of our new model in the geophysical limit where one phase, called the "fluid" phase, is much less viscous than the other phase, named the "matrix" phase; mathematically $\mu_f \ll \mu_m$, where μ is the shear viscosity and the indices f and m denote the fluid and the matrix, respectively. This approximation largely simplifies the equations. In the following the model will be applied to problems of melting and melt migration and planetary differentiation. The fluid phase is either a basaltic magma ($\mu_f \sim 10\,\mathrm{Pa\,s}$) or liquid iron alloy ($\mu_f \sim 0.1\,\mathrm{Pa\,s}$) and the matrix phase is silicate rock ($\mu_m \sim 10^{20}\,\mathrm{Pa\,s}$). The approximation of a large viscosity difference is therefore justified. The general set of equations as well as the detailed derivation can be found in the thesis manuscript.

The conservation of mass in each of the phases writes

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot (\phi \mathbf{v}_f) = \frac{\Delta\Gamma}{\rho_f}, \tag{1}$$

$$-\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot [(1-\phi)\mathbf{v}_m] = -\frac{\Delta\Gamma}{\rho_m}, \tag{2}$$

where ϕ is porosity, the volume fraction of the fluid phase, ρ_f and ρ_m are the densities which are uniform and constant, and $\mathbf{v}_f$ and $\mathbf{v}_m$ are the averaged velocities of the fluid and matrix phase. The source terms on the right-hand sides are proportional to the melting rate $\Delta\Gamma$.

The equations that express the balance of forces acting on each of the phases are the generalized Darcy's law

$$-\boldsymbol{\nabla} P_f + \rho_f \mathbf{g} + \frac{c\boldsymbol{\Delta}\mathbf{v}}{\phi} = 0, \tag{3}$$

and the equation of matrix deformation

$$-(1-\phi)(\boldsymbol{\nabla} P_m - \rho_m \mathbf{g}) + \boldsymbol{\nabla} \cdot [(1-\phi)\underline{\boldsymbol{\tau}}_m] - c\boldsymbol{\Delta}\mathbf{v} + \Delta P \boldsymbol{\nabla}\phi + \boldsymbol{\nabla}(\sigma\alpha) = 0, \tag{4}$$

where P_f and P_m are the fluid and matrix pressures, $\Delta P = P_m - P_f$ is the pressure difference, $\mathbf{g}$ is the acceleration of gravity, and $\boldsymbol{\Delta}\mathbf{v} = \mathbf{v}_m - \mathbf{v}_f$ is the difference in average velocities. In the limit of inviscid fluid the interfacial surface force $\boldsymbol{\nabla}(\sigma\alpha)$ acts only on the matrix; σ is the coefficient of surface tension and α is the interfacial area density (interfacial surface per unit volume).

The coefficient c that scales the friction between the two phases moving at different velocities, is related to the porosity-dependent permeability of the Darcy's law (Darcy, 1856) by

$$c = \frac{\phi^2 \mu_f}{k(\phi)}. \tag{5}$$

The deviatoric stress in the matrix is

$$\boldsymbol{\tau}_m = \mu_m \left(\boldsymbol{\nabla} \mathbf{v}_m + [\boldsymbol{\nabla} \mathbf{v}_m]^T - \frac{2}{3} \boldsymbol{\nabla} \cdot \mathbf{v}_m \underline{\mathbf{I}} \right), \tag{6}$$

where $\underline{\mathbf{I}}$ is the identity tensor and $[\ ]^T$ denotes a tensor transpose. We need to emphasize that even though the matrix (as well as the fluid) are individually incompressible, the divergence of the average matrix velocity is not identically equal to zero. A non-zero $\boldsymbol{\nabla} \cdot \mathbf{v}_m$ reflects a rate of isotropic deformation – that is, the dilation (if positive) or compaction (if negative) of the matrix skeleton. Even with only one viscosity present in equation (6), $\underline{\boldsymbol{\tau}}_m$ is not a stress tensor of an incompressible fluid but a deviatoric stress proportional to the rate of shear (non-isotropic) deformation.

The non-equilibrium thermodynamics considerations on the entropy production, in particular the requirements of the second law of thermodynamics, the use or Onsager's relations and consideration of various micro-mechanical pore/grain deformation models, constrain two phenomenological relations. One of them is an equation for the pressure difference

$$\Delta P = -\sigma \frac{\mathrm{d}\alpha}{\mathrm{d}\phi} - \frac{\mu_m}{\phi} \boldsymbol{\nabla} \cdot \mathbf{v}_m. \tag{7}$$

The first term on the right is the static pressure difference due to surface tension on a curved interface (the derivative $\mathrm{d}\alpha/\mathrm{d}\phi$ represents the sum of the principal curvatures; Bercovici *et al.*, 2001a). The second term is the dynamic pressure difference due to compaction/dilation of the matrix. The porosity dependent factor μ_m/ϕ plays the role of the bulk viscosity of some previous two-phase models (e.g., Schmeling, 2000).

The other phenomenological relation is an equation for the melting rate in a univariant system (i.e., one containing a single component in two phases)

$$\Delta\Gamma = -\chi \left[(T - T_0)\Delta s + P_f \frac{\Delta\rho}{\rho_f \rho_m} + \frac{\sigma}{\rho_m} \frac{\mathrm{d}\alpha}{\mathrm{d}\phi} \right], \tag{8}$$

where T is temperature (we assume local thermal equilibrium, therefore the same temperature in both phases) and $\Delta s = s_m - s_f$ is the difference in specific entropies. The melting curve is given by its slope $\mathrm{d}T/\mathrm{d}P_f|_{fus} = -\Delta\rho/(\rho_f \rho_m \Delta s)$ and is fixed at a temperature T_0 at ambient pressure in the absence of surface tension. This is a kinetic relation where the melting is proportional to the departure from thermodynamic equilibrium (the big bracket on the right) through a kinetic coefficient χ. Alternatively, one can consider an equilibrium phase change. This corresponds to a very large ("infinite") coefficient χ and the expression in the big bracket equal to zero, together giving a finite melting rate.

The energy equation is

$$\rho_f \phi C \frac{\mathrm{D}_f T}{\mathrm{D}t} + \rho_m (1-\phi) C \frac{\mathrm{D}_m T}{\mathrm{D}t} - T\Delta s \Delta\Gamma$$
$$= Q - \boldsymbol{\nabla} \cdot \mathbf{q} + \frac{\Delta\Gamma^2}{\chi} + c\boldsymbol{\Delta}\mathbf{v}^2 + K_0 \mu_m \frac{1-\phi}{\phi} (\boldsymbol{\nabla} \cdot \mathbf{v}_m)^2 + (1-\phi)\underline{\boldsymbol{\tau}}_m : \boldsymbol{\nabla} \mathbf{v}_m, \tag{9}$$

where C_f and C_m are specific heats, Q is the power of volumetric heat sources, $\mathbf{q}$ is the heat flux ($\mathbf{q} = -k_T \boldsymbol{\nabla} T$, k_T is the coefficient of thermal conductivity).

The third term on the left is the energetic contribution of phase change; $-T\Delta s$ is the specific latent heat which is multiplied by the melting rate in equation (9). On the right-hand side, aside from the trivial heat sources, there are three dissipative sources:

- due to friction between the phases which move at different velocities (the term proportional to Δv^2),
- due to the isotropic deformation of the matrix (the term proportional to $(\boldsymbol{\nabla}\cdot\mathbf{v}_m)^2$),
- due to the shear deformation of the matrix (the last term),

and another heat source proportional to the square of the melting rate; this last one disappears if melting takes place in equilibrium.

We now have a consistent set of coupled two vector equations (3, 4) and five scalar equations (1, 2, 7–9), for two velocity fields ($\mathbf{v}_f$ and $\mathbf{v}_m$) and five scalar quantities (ϕ, P_f, P_m, T and $\Delta\Gamma$), supplemented with the rheological relation (6). To our knowledge this is the first geophysical model where two-phase flow and deformation and melting are properly coupled.

4 Metal–silicate differentiation

We use the two-phase model to investigate the dynamics of metal–silicate differentiation on a planetary scale, which took place in the young terrestrial planets. The differentiation is primarily driven by the density contrast between the lighter silicate component and the more dense metallic components (Fe–FeS alloy). The release of gravitational energy by differentiation contributes an important heat source to the energy balance and is accounted for in our model. We investigate the case where the silicate component is in the solid state and the metallic component may be molten. Such a situation is a plausible intermediate physical state between the cases of both components in molten state (i.e., the presence of a magma ocean) and a solid–solid phase separation, as the melting temperature of the metallic component is lower than that of the silicates (Agee *et al.*, 1995). There is no transfer of mass between the metallic and the silicate components in our current model.

First we present the equations for compaction, phase separation and two phase convection in a way that is appropriate to develop a numerical code. We discuss the modification for a case where the metallic component is either in the solid or in the liquid state. Calculations of a compaction in a layer and self-gravitating spherically symmetric body are presented. These 1-D calculations suggest a rather short time scale of differentiation. For a protoplanet of 1600 km of radius and assuming that the metallic phase is molten, the protocore can form in ~ 10 kyr.

We then develop a numerical model of two-phase convection and phase separation in two-dimensional case in Cartesian geometry. In 2-D, we cannot take into account the self-gravitation (i.e., the fact that gravity changes during differentiation) and we simply assume the gravity to be uniform and constant. The velocity field contains both the incompressible flow component and the compressible (irrotational) flow; the interaction between convection and compaction is therefore included.

We show simulations of metal–silicate segregation triggered by an impact which was a common event during the late stage of planetary accretion (Wetherill, 1985): at the initial time, we increase the temperature in a circular zone close to the surface so that the temperature becomes higher than the melting temperature of iron, while it is below the melting temperature elsewhere. Figure 1 shows the evolution of the metal volume fraction for one calculation. Several stages of different prevailing segregation mechanisms can be identified in the simulation run. Initially the circular zone, containing molten metallic phase, segregates by a roughly 1-D porous flow. The molten metal concentrates and the iron content increases to a value close to 1. The dense metallic blob eventually descends in a diapir-like fall while the light residual silicate mantle rises and starts spreading along the surface. When the metal reaches the bottom it spreads as a gravity current and forms a protocore. Along the cusp-like channel that connects the differentiated silicates to the core pockets of metal form and descend to the protocore. The gravitational energy released by the formation of the increasingly layered differentiated structure is converted into heat and increases the temperature. The local temperature rise can induce further melting of the metallic phase and thus facilitate further segregation. At the interface between the differentiated silicate and the remaining undifferentiated mantle new metallic ponds are formed that trigger new instabilities. These secondary instabilities follow the same kind of dynamics that the initial one with cusp-like channel connecting them to the surface. The same process (creation of metallic ponds and descent of diapirs) occurs again. Large undifferentiated islands survive for some time and are slowly eroded until the whole planet is differentiated. During the whole process various compaction waves are visible in both the silicates and the core.

Our model accounts for a spectrum of proposed planetary differentiation mechanisms. The increase of temperature due to segregation (release of gravitational energy) is comparable to the initial heat delivered by the impact so that the process of segregation, once started, is more or less self maintained. The first diapir that crosses the mantle leaves a cusp-like trail that connects the protocore to the near surface silicates across the undifferentiated material. Melting occurs continuously both in the shallow and in the deep mantle. The sinking of metallic diapirs is very fast (of order of 10 kyr for a protoplanet of 1600 km in radius) as instead of deforming the surrounding material as in a usual Stokes flow, the undifferentiated material desegregates on the bottom side of the diapir, the silicates cross the metallic phase, and accumulate behind the sinking diapir. The first impact that melts the iron phase is therefore potentially able to trigger the whole core–mantle segregation. For a protoplanet of 1600 km in radius the whole differentiation process is completed in few hundred kyr.

5 Coupling between compaction and melting

With our novel set of equations of two-phase flow where deformation and melting are coupled, we can investigate the effect of viscous deformation on the phase change. We have shown how the compaction of the matrix induces a difference of pressures between the solid and the melt (equation 7). The pressure dependent melting temperature is therefore modified when the solid deforms. We analyze a simple 1-D melting problem. Similar problems were discussed by McKenzie (1984), Ribe (1985) and Turcotte & Phipps Morgan (1992). Although some of these studies described simultaneous melting and compaction, they did not account for the feedback between the viscous deformation and the thermodynamics of melting.

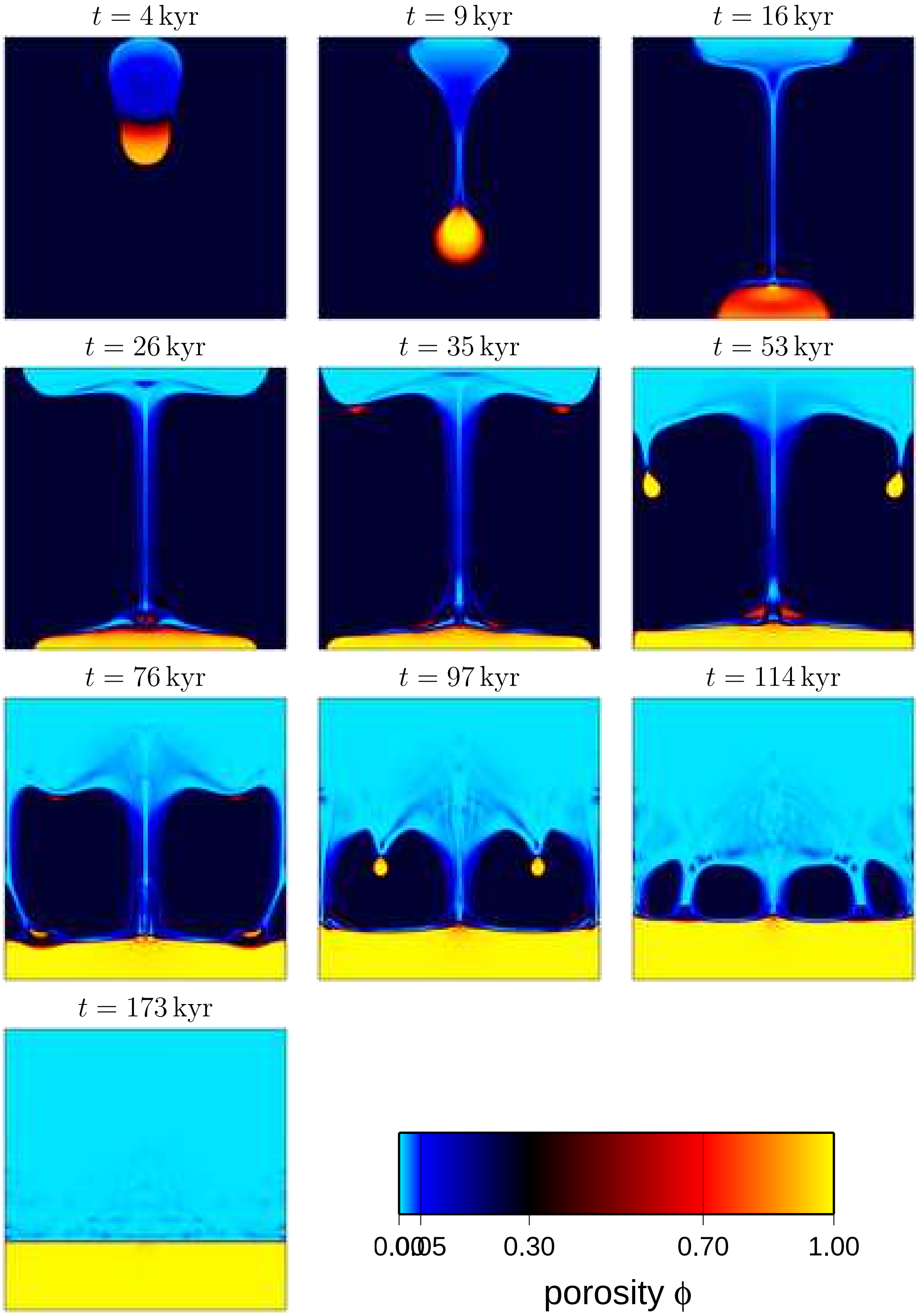

Figure 1: Evolution of the volume fraction of metal (porosity) after an impact in a square box calculation with an initially uniform metal distribution. A circular zone of radius equal to 1/6 of the box size is initially heated above the melting temperature of the iron phase. The color scale is such that the pure metallic phase is yellow, the pure silicate phase is cyan and the undifferentiated mantle is black. The box is mass conserving, thermally insulated, with free slip condition at the boundary.

In our model we consider melting in a univariant system. In the melting region temperature follows the Clapeyron slope, which describes the equilibrium between the phases. Melt extraction, which occurs simultaneously with melting, leads to viscous deformation of the matrix and consequently to different pressure fields in the two phases. The matrix material initially ascends with an upward velocity V. No heat is supplied to the ascending matrix; before melting begins, the solid ascends adiabatically, and in fact isothermally as the matrix is incompressible. The melting starts when the ascending solid reaches the melting pressure. From this point on two phases coexist until all the matrix has melted (we consider complete melting). Above the melting zone, melt is transported isothermally again. We are primarily interested in the effect of deformation on melting and neglect surface tension. We investigate the steady-state solution of this problem.

In the partially molten zone three forces are in balance:

$$\delta^2 \phi \frac{\mathrm{d}}{\mathrm{d}z} \left(\frac{1-\phi^2}{\phi} \frac{\mathrm{d}v_m}{\mathrm{d}z} \right) - \Delta v = V_B \phi (1-\phi); \tag{10}$$

this equation is obtained by a linear combination of (3) and (4). The first term represents the viscous forces due to matrix deformation; it is scaled by the square of the compaction length $\delta = \sqrt{4\mu_m/(3c)}$. The second term on the left is the Darcy drag due to friction between the solid and the melt moving at a different velocity. The term on the right is the buoyancy forcing of the melt extraction; $V_B = \Delta\rho g/c$ is the buoyancy velocity.

In magmatic settings the compaction length is typically much smaller than the thickness of the melting zone. On this basis, most previous studies used the so called "Darcy approximation" where the compaction length is put equal to zero. In that case there is a simple balance between the buoyancy and the Darcy friction in the melting zone, and the whole system of equations greatly simplifies. We show however, that the Darcy equilibrium approximation is not valid near the incipient melting (that is, at a very small porosity). In fact, we have identified various possible regimes of force balance in the melting zone. Figure 2 summarizes these various domains. Near the incipient melting there is a region where the buoyancy is weak and where the Darcy friction is counteracted by the viscous forces. The Darcy equilibrium is only valid at certain distance above the depth of first melting. With parameters appropriate for melting under an oceanic spreading center ($\delta \sim 10\,\mathrm{km}$, $V_B \sim 100V$; V is the initial upwelling velocity below the melting zone) the thickness of this boundary domain is few kilometers. If the compaction length is comparable to the melting zone size (not the case for melting beneath oceanic spreading centers, though), a different regime is possible where the Darcy drag can be neglected.

Figure 3 shows the porosity and velocity profiles in the melting zone. The porosity is an increasing function of the vertical coordinate and the porosity remains much smaller than the degree of melting, which is roughly linear between 0 and 1 across the melting zone. Even at a degree of melting close to 1, porosity remains below 10 %. This contradicts the batch melting models where the porosity and the degree of melting are comparable. At the end of the melting zone the melt accumulates rapidly and porosity reaches 1. The matrix velocity monotonically decreases as melting proceeds. The velocity of the lighter magma increases and reaches about $10V$ (ten times the initial velocity of the upwelling). We find that the deformation of the solid matrix at the incipient melting

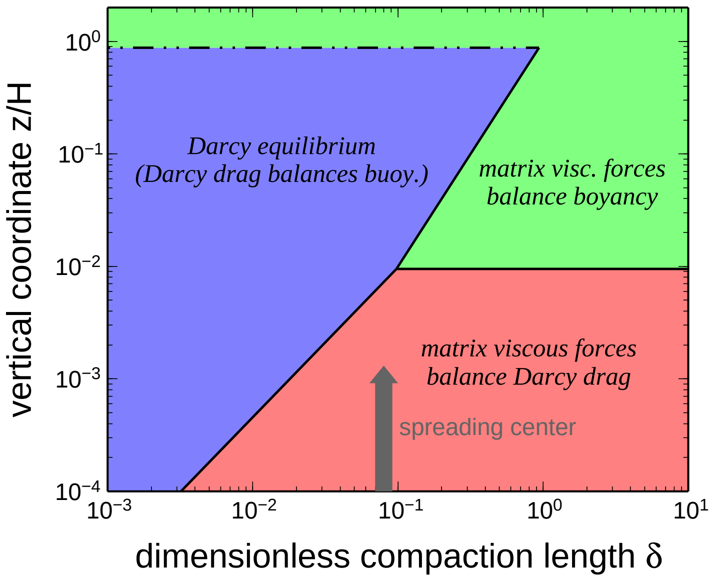

Figure 2: Graphical representation of the various regions along the melting zone as a function of the dimensionless compaction length $\delta' = \delta/H = \sqrt{4\mu_m/(3cH^2)}$ (on horizontal axis with logarithmic scaling; $H = 115\,\mathrm{km}$ is the vertical extent of the partially molten zone). The dimensionless vertical coordinate $z' = z/H$ is plotted on the vertical axis in logarithmic scale, melting starts at $z = 0$. Plotted for dimensionless buoyancy velocity $V_B' = V_B/V = \Delta\rho g/(cV) = 60$. The compaction length appropriate for melting under a ridge is indicated by an arrow.

results in elevation or depression of the melting zone with respect to predictions based on the average pressure. The model suggests that for $V_B \gtrsim V$, melting begins deeper than standard Clapeyron slope predicts; likewise for $V_B \lesssim V$, melting does not begin until lower pressure is reached. Below an oceanic ridge, melting can begin a few km deeper than what one would infer from the average pressure. The pressure difference due to matrix deformation exists all along the melting zone and is of the order of 5 MPa.

6 Summary and conclusion

The presented thesis is concerned with the mechanical and thermodynamical modeling of two-phase flow, an important phenomenon in the Earth's interior. In the thesis we derive in a rigorous fashion a set of equations describing the two-phase dynamics in the presence of phase change. Our model properly accounts for the feedback between the viscous deformation of the phases and the thermodynamic conditions of melting/freezing. Following previous work (Bercovici *et al.*, 2001a; Ricard *et al.*, 2001; Bercovici & Ricard, 2003), we account for the presence of surface tension on the interface between the two phases which imposes a clear distinction between the properties of each phase and those of the interface (pressures, velocities and densities). The conditions of equilibrium between the two phases are naturally deduced from the second law of thermodynamics. The usual Clapeyron slope is affected by the presence of the surface tension (Gibbs-Thomson effect) and by the dynamic pressure difference between the phases. This pressure difference is proportional to the rate of matrix compaction and to the inverse of porosity. It is only

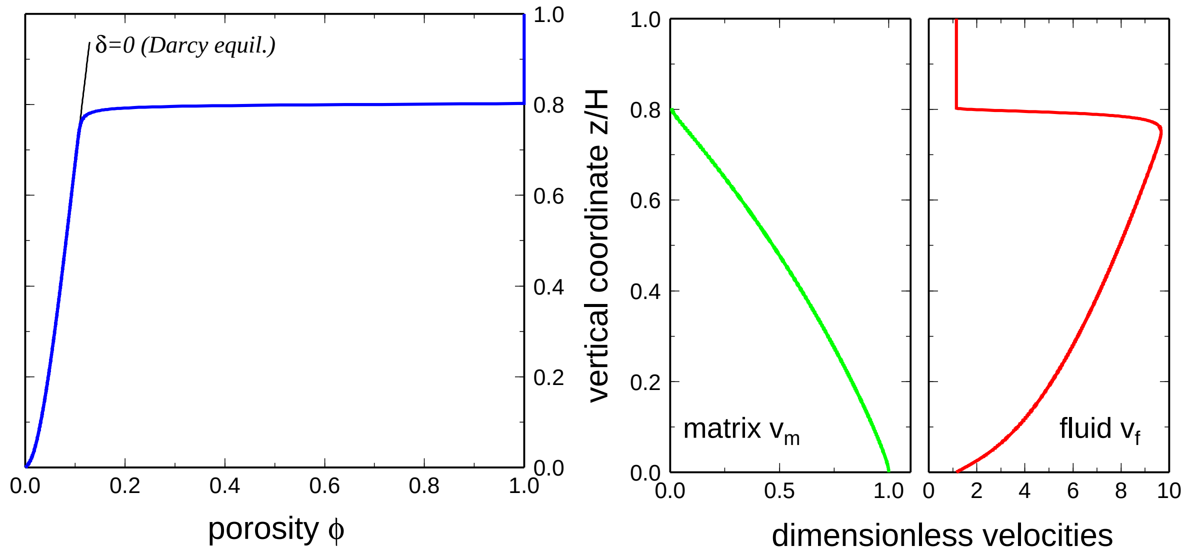

Figure 3: Porosity ϕ, matrix velocity v_m and fluid (magma) velocity v_f in the melting zone. Velocities are scaled with the initial upwelling velocity V. Calculated with $\delta = 30\,\text{km}$ and $V_B = 100V$. Porosity in Darcy equilibrium ($\delta = 0$) is shown as thin dotted line.

in the case of motionless mixture without surface tension that the usual Clapeyron slope is recovered. In the motionless case with surface tension, the pressure difference between the phases verifies the Laplace's condition but the phase equilibrium is affected by the Gibbs-Thomson effect. The model also allows for non-equilibrium situations, in which case a kinetic relation links the melting rate to the departure from equilibrium.

We present models of planetary core–mantle differentiation. In particular we have developed a 2-D Cartesian model of two-phase circulation and compaction that accounts for the conversion of gravitational energy into heat. Our simulations show that the temperature increase upon impact on a growing planet can trigger a segregation instability that results in the differentiation of the initially uniform body. Several differentiation mechanisms are observed in the simulations (quasi-1D segregation, Rayleigh-Taylor instability, diapiric flow, gravity current spreading) where molten metal separates from solid silicates.

We studied the effect of the solid matrix compaction on melting in a 1-D model of equilibrium pressure release melting. The matrix deformation generates a dynamic pressure difference between the solid and the melt; the magma is submitted to lower pressure than the compacting matrix. This effect is particularly important at the incipient melting where it depresses the base of the melting zone by few km. The effect of surface tension on melting is also discussed and depends on the energy balance of the interfaces at the grain scale, and consequently on the geometry of the first melt. The magma extraction velocities reach up to ten times the initial upwelling velocity and the porosity remains small ($\lesssim 10\,\%$) in the entire melting zone.

The present theory offers a framework for treatment of physical situations where two-phase flow with phase change is concerned. Although our focus was on geological settings, the description is relevant to much wider spectrum of applications (such as, for example, various problems involving granular media, transport of water/oil/gas in porous media, metal alloys, mechanics of soils and sediments). The presented applications represent a work in progress. Several obvious extensions to what is discussed in the present thesis are possible, including more realistic simulations of planetary differentiation and thermal evolution, melting of multivariant material, non-equilibrium time-dependent melting, and 2-D (3-D) flow modeling in specific geological settings.

Acknowledgments

I would like to express my sincere gratitude to all the people who made the completion of this thesis possible. My biggest thanks go to Yanick Ricard for his guidance, invaluable advice and help, his encouragement throughout the writing process and his friendship over those five years that we have been working together. I thank David Bercovici who I had the privilege to work with at Yale University, for the numerous excellent scientific discussions and for his support both on professional and personal level. Thanks to Ondřej Čadek for his help in Prague. I am grateful to many people who I interacted with at the three departments where I have worked – in Lyon, at Yale and in Prague, who have, in one way or another, contributed to my professional development, who created a stimulating and friendly environment to work in. The long list contains my fellow grad students, postdocs, research personnel, faculty, as well as the staff of the departments. On a personal note, I thank my family, my friends and my partner Lisa for their generous support and caring.

The electronic version of this document, as well as the thesis manuscript and other materials can be found at `http://geo.mff.cuni.cz/~sramek/thesis/`.

References

Agee, C. B., Li, J., Shannon, M. C. & Circone, S., 1995. Pressure-temperature phase diagram for the Allende meteorite, *J. Geophys. Res.*, **100**(B9), 17725–17740.

Ahern, J. L. & Turcotte, D. L., 1979. Magma migration beneath an ocean ridge, *Earth Planet. Sci. Lett.*, **45**(1), 115–122.

Bercovici, D. & Ricard, Y., 2003. Energetics of a two-phase model of lithospheric damage, shear localization and plate boundary formation, *Geophys. J. Int.*, **152**(3), 581–596.

Bercovici, D. & Ricard, Y., 2005. Tectonic plate generation and two-phase damage: Void growth versus grain size reduction, *J. Geophys. Res.*, **110**(B3), B03401.

Bercovici, D., Ricard, Y. & Schubert, G., 2001a. A two-phase model for compaction and damage, Part 1: General theory, *J. Geophys. Res.*, **106**(B5), 8887–8906.

Bercovici, D., Ricard, Y. & Schubert, G., 2001b. A two-phase model for compaction and damage, Part 3: Application to shear localization and plate boundary formation, *J. Geophys. Res.*, **106**(B5), 8925–8939.

Darcy, H., 1856. Les fontaines publiques de la ville de Dijon, Dalmont, Paris.

Drew, D. A. & Passman, S. L., 1998. *Theory of Multicomponent Fluids*, vol. 135 of *Applied Mathematical Sciences*, Springer-Verlag, New York.

McKenzie, D., 1984. The generation and compaction of partially molten rock, *J. Petrol.*, **25**(3), 713–765.

Ribe, N. M., 1985. The deformation and compaction of partial molten zones, *Geophys. J. Roy. Astron. Soc.*, **83**(2), 487–501.

Ricard, Y., Bercovici, D. & Schubert, G., 2001. A two-phase model for compaction and damage, Part 2: Applications to compaction, deformation and the role of interfacial surface tension, *J. Geophys. Res.*, **106**(B5), 8907–8924.

Schmeling, H., 2000. Partial melting and melt segregation in a convecting mantle, in *Physics and Chemistry of Partially Molten Rocks*, eds. N. Bagdassarov, D. Laporte & A. B. Thompson, vol. 11 of *Petrology and Structural Geology*, chap. 5, pp. 141–178, Kluwer Academic Publisher, Dordrecht.

Sleep, N. H., 1974. Segregation of magma from a mostly crystalline mush, *Geol. Soc. Am. Bull.*, **85**(8), 1225–1232.

Šrámek, O., Ricard, Y. & Bercovici, D., 2007. Simultaneous melting and compaction in deformable two-phase media, *Geophys. J. Int.*, **168**(3), 964–982.

Turcotte, D. L. & Ahern, J. L., 1978. Porous flow model for magma migration in the asthenosphere, *J. Geophys. Res.*, **83**, 767–772.

Turcotte, D. L. & Phipps Morgan, J., 1992. The physics of magma migration and mantle flow beneath a mid-ocean ridge, in *Mantle Flow and Melt Generation at Mid-Ocean Ridges*, eds. J. Phipps Morgan, D. K. Blackmann & J. M. Simpson, AGU Geophysical Monograph 71, pp. 155–182, American Geophysical Union, New York.

Wetherill, G. W., 1985. Occurrence of giant impacts during the growth of the terrestrial planets, *Science*, **228**(4701), 877–879.