Report on the thesis

Equilibration between sinking metal droplets and molten silicates in magma oceans

submitted by Martina Ulvrová

to the Department of Geophysics, Faculty of Mathematics and Physics, Charles University in Prague, for the degree of Master ("Mgr.")

Reviewer:

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Ms. Ulvrová's thesis is concerned with the modeling of chemical equilibration of liquid metal particles in molten silicates. This is an important problem relevant to the early evolution of the Earth, when extensive, possibly global magma ocean(s) existed. In these magma oceans the heavier metallic iron phase separated from the lighter silicates in the form of droplets. The aim of the thesis is to investigate the kinetics of equilibration of dispersed metallic droplets falling in silicate magma. This is done by considering an advection-diffusion problem for the trace element concentration in a single spherical droplet during its fall. The problem is set up in the reference frame of the falling droplet, where the spherically symmetric geometry can be exploited. The material parameters (density, viscosity, diffusion coefficient) differ between the inner domain (the iron droplet) and the outer domain (silicate liquid). The spherical interface between domains is impermeable (zero normal velocity), but allows for the diffusion of the trace element. A constant terminal velocity of the sinking and the corresponding steady-state velocity fields in both the droplet and the silicate are assumed. The problem thus translates into a solution of two time-dependent advection-diffusion equations – one in each domain, coupled through the boundary condition at the interface, where an equilibrium concentration ratio (the partition coefficient) and continuity of trace element diffusive flux are prescribed.

After the introduction in Chapter 1, the physical model is described in Chapter 2. In section 2.1 the advection-diffusion equation is presented, the geometry of the model is shown in Section 2.2, and the boundary conditions are discussed in Section 2.3. The velocity fields in both the inner and the outer domains are derived in Section 2.4; to my understanding, this represents a re-derivation of previously known results and this should be clearly stated at the beginning of the section. In Section 2.5 the advection-diffusion equations are presented in the dimensionless form and three dimensionless controlling parameters are identified: the Péclet number, the ratio of viscosities and the ratio of diffusion coefficients. Section 2.7 discusses the relevant values of the model parameters. In Section 2.6 an approximate analytical solution is found, which predicts an exponential decrease, with time, of the average concentration in the metal droplet, where the characteristic equilibration time is proportional to the partition coefficient and to a positive power of the number. The result is obtained for both a finite viscosity of the metallic droplet and a rigid sphere. Chapter 3 describes the finite-volume numerical code developed by the author. The equations are resolved in a spherical domain twice the radius of the droplet, where the external boundary conditions are chosen to approximate an infinite medium. Some basic benchmarks are performed. In Chapter 4, the results of numerical experiments are presented, equilibration times are determined and compared to the analytical results. Ranges of the Péclet number and viscosity ratio values are explored. Two different regimes are found for small (<1) and large (>100) ratio of iron to silicate viscosity, for which the dependence of equilibration time on the Péclet number is well explained by the analytical model. The present analysis is limited to a single value of the partition coefficient and of the ratio of diffusion coefficients; it would be interesting so see the validity threshold of the analytical result in terms of the latter parameter. As discussed in Chapter 5, the results suggest fast (shorter than sinking time in the magma ocean) equilibration for slightly siderophile elements. For moderately to highly siderophile elements the degree of equilibration depends on the viscosity of the silicates.

Ms. Ulvrová's fluid mechanical treatment, that includes both advection and diffusion inside the metallic droplet, represents an important improvement of the falling sphere equilibration model with respect to previous works, which only considered diffusion in the droplet. The mathematical model is properly set up and Ms. Ulvrová demonstrates her expertise by finding an analytical solution and developing a fine numerical code. More room could be devoted to a discussion of the physical implications of the results in reference to the Earth. Regarding the form, the language is often awkward and difficult to read. The manuscript would largely benefit from a thorough editorial review; this concerns the grammar, phrasing, word choice, and occasional spelling mistakes and inconsistencies.

In conclusion, Ms. Ulvrová's thesis presents significant original results and I encourage their publication in a peer-reviewed journal, possibly after extending the analysis (as suggested in the concluding Chapter 6) and discussion. I judge that the thesis justifies the award of the Master's ("Mgr.") degree and suggest the grade "výborně".

Comments on the manuscript (please, address ★-comments at the defense):

- p.6, first paragraph: Models of core formation were surely suggested earlier than late 1980's
- p.6, third paragraph: The claim about coefficient of surface tension values deserves a citations; moreover, only comparing iron and water is not very informative
- ★p.9: The first time *concentration* is mentioned, its units should be specified (concentration can be defined many different ways). What are the units of concentration used here?
- ★p.10, above Eq2.4: The particles cannot both enter and leave the volume on average. Is Q defined as inflow or outflow?
- p.11: I think that "no-material boundary" is not an established (defined) term.
- caption of Fig 2.2 (p.17): As there is no scale bar (a) or isolines increments specified (b) in the figures, the only relevant parameter that needs to be mentioned is the viscosity ratio (later defined as R_μ). In fact, from the specified values and using Eq. 2.54 one gets $|\varrho^{I}-\varrho^{II}|g=15/4$ in SI units, which is clearly unreasonable for the problem considered.
- Fig 2.3 (p.17): This figure better have R_μ on the horizontal axis – then a single curve covers everything (R_U is only a function of R_μ)
- p.18, first paragraph: should be "...use the initial concentration *in the metallic droplet*" (or something similar)
- p.19, Eqs2.70,2.71: on the right side, a characteristic concentration magnitude C_2-C_1 should be present instead of C^{II}
- p.19, step from Eq2.64 to Eq2.73: the change of variables should be either shown in detail or a reference offered
- p.20, after Eq2.75: About 2 pages were dedicated to setting up the analytical model and the reader should be rewarded with the explicit solution to Eq2.73.
- p.20, after Eq2.75: I_{liq} is not well defined.
- p.25, first paragraph: Boundary condition 2.14 is also part of the system.
- ★p.25, 4th phrase in Sec3.1: "As the flux..." The statement is wrong. Please, rectify.
- p.27, Eq3.6, second line: dr shoud be Δr
- p.27, Eq3.7, first line: $d\theta$ should be $\Delta\theta$
- p.26–31: Strictly speaking, the fluxes F and surface elements S should all carry both j- and k- indices. The velocities v_r and v_θ should also carry j,k-indices.
- Fig3.2 (p.30): In the caption "Vertical" should be "Horizontal"
- p.31, Eq3.26: $d\theta$ should be $\Delta\theta$
- p.31, Eq3.27: $C^{II}_{JMAX,k-1}$ and $C^{II}_{JMAX,k-2}$ should carry an asterisk
- p.31, last phrase in Section 3.4: "Despite..." What is meant by that? For very small diffusion coefficient it is obvious that the time stepping is limited by the advective term (why "despite"?).
- p.47: In spherically symmetric case, the right sides of A.6 and A.7 should be zero. In fact, Eqs A.6–A.8 are not used.

Questions for discussion (please, be prepared to answer any of them):

- Can you show that the boundary layer thickness is $\sim(DR/U)^{1/2}$? (p.11, second par.)
- ★The analytical model presented in section 2.6 contains several strong assumptions:
  1) assumption of a thin boundary layer near the interface in the outer domain
  2) in particular, neglect of the angular part of the Laplacian in Eq.2.64
  3) uniform concentration in the metallic droplet at all times

  What do these assumptions mean in terms of physical processes that take place in the two domains?
  Are there some values of the model parameters (of a combination of several of them), for which these assumptions do not hold? Is this confirmed by the numerical solution?
- Can you show how the Weber number is obtained? (that is, show and explain the scaling of the two quantities representing the inertia and surface tension; Eq2.84)
- ★The benchmark described in Section 3.5.1 only tests the radial part of the Poisson equation. Have you performed any tests that involve the angular part?
- ★When benchmarking the advection scheme, you mention some numerical oscillations. Can you comment more on that? What is their origin? Also, you mention (Section 3.4) that Courant numbers greater that one are used without loosing the scheme's stability. Does the solution remain accurate?
- ★How can your results help in understanding or explaining the current concentration of siderophile element in Earth's mantle? Also, can you briefly comment on your work in relation to other studies on the kinetics of metal–silicate equilibration?

Prague, 26 May 2008

[redacted]