



Assessing uncertainty in geochemical models for core formation in Earth



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ABSTRACT

Unraveling the conditions at which Earth's metallic iron core formed yields important information about Earth's early accretion and differentiation history. Multi-variable statistical modeling of siderophile element partitioning between core-forming metallic liquids and silicate melts form the basis for physical models of core formation. While it seems clear that core segregation in a deep peridotitic magma ocean is generally consistent with many mantle siderophile element abundances, there is considerable disparity among extant physical models in terms of the key parameters of pressure, temperature and oxygen fugacity at which the core formed. Moreover, there is ongoing debate over whether simple single-stage equilibrium or more complex multi-stage accretion models are required by the partitioning data. Here we consider how variations in the statistical regression of partitioning data affect the outcomes of physical models for core formation. Taking extant experimental data sets for four well-studied siderophile elements (Ni, Co, W and V) as examples, we find that the regression model exerts a fundamental control on physical model outcomes. Further, the experimental data are currently too imprecise to discriminate among various single-stage and continuous core formation scenarios. Progress in the development of physical models requires better isolation of the independent variables that affect partition coefficients and verification of activity models at high pressure and temperature in order to reduce the global uncertainty in multi-variable statistical models.

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1. Introduction

Models of core formation in Earth have historically been designed around the concept of segregation of a core-forming metal from a silicate mantle (Ringwood, 1966). The modern view of planetary accretion by energetic impacts among proto-planets implies that segregation and equilibration occurred when both phases were molten, probably within a deep magma ocean (Benz and Cameron, 1990; Canup, 2004; Chambers, 2004; Melosh, 1990; Tonks and Melosh, 1993). In principle, if the partitioning behavior of siderophile elements between metal and silicate are known, the conditions of equilibrium core formation can be deduced and important constraints placed on early Earth processes. The objective is to find a unique or progressive set of conditions of pressure, temperature, oxygen fugacity, and silicate melt and metal composition that can account for the observed mantle abundance of a suite of siderophile elements (see reviews by Righter (2003), Walter et al. (2000), Wood et al. (2006)). In practice, this requires high pressure and temperature experiments that equilibrate liquid metal with molten silicate, the accurate and precise analysis of siderophile elements in both phases, and a statistical

model that parameterizes the partitioning behavior and provides a measure of model uncertainty.

Currently there are many competing physical models for the origin of the siderophile element signature of Earth's mantle (Chabot et al., 2005; Corgne et al., 2008, 2009; Cottrell et al., 2009; Hillgren et al., 1994; Kegler et al., 2008; Li and Agee, 1996, 2001; Mann et al., 2009; Righter, 2011a; Righter and Drake, 1999; Righter et al., 1997; Rubie et al., 2011; Siebert et al., 2012, 2011; Thibault and Walter, 1995; Wade and Wood, 2005; Walter and Tronnes, 2004; Wood et al., 2008). Here we will limit our discussion to the two dominant paradigms, both of which require metal–silicate equilibration in a deep magma ocean. In the simplest single-stage core formation scenario, the metal and silicate are assumed to have equilibrated at some average high pressure and temperature, possibly at the base of a deep magma ocean, (e.g. Corgne et al., 2009; Cottrell et al., 2009; Li and Agee, 1996, 2001; Mann et al., 2009; Righter, 2011a; Righter and Drake, 1999; Righter et al., 1997; Walter and Tronnes, 2004). In multi-stage or continuous accretion models, the magma ocean conditions evolve as the planet accretes with progressively changing conditions of variables such as pressure, temperature and oxygen fugacity (e.g. Corgne et al., 2008; O'Neill, 1991; Siebert et al., 2011; Wade and Wood, 2005; Wood et al., 2008, 2006). Even though the number of elements included in models and the availability of experiments has grown considerably, there is

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currently little consensus among studies regarding the conditions or mode of core formation required by the experimental data, except that high pressure and temperature equilibration is strongly implicated.

A good example is the current debate over whether or not single-stage core formation models are viable, or whether continuous accretion with progressively changing pressure, temperature and oxygen fugacity are a requirement of the partitioning data (Corgne et al., 2008, 2009; Cottrell et al., 2009; Righter, 2011a; Siebert et al., 2011; Wade and Wood, 2005; Wood et al., 2008, 2006). In several studies it is argued that single-stage models are not viable because the mantle abundances of specific elements, and most notably vanadium (V), cannot be reconciled with available partitioning data for equilibration along the liquidus or solidus in a deep magma ocean at an oxygen fugacity corresponding to a mantle with ~ 6.3 wt% Fe (Corgne et al., 2008; Siebert et al., 2011; Wade and Wood, 2005; Wood et al., 2008, 2006). In contrast, Righter (2011a) has argued using effectively the same data sets and elements that continuous accretion with progressive oxidation is not a unique requirement of the data, and that single-stage models are viable and perhaps even the preferred solution.

Some authors have estimated the uncertainty in physical models for core formation (Chabot et al., 2005; Corgne et al., 2008, 2009; Cottrell et al., 2009; Li and Agee, 2001; Righter, 2011a; Righter and Drake, 1999; Righter et al., 1997; Rudge et al., 2010; Siebert et al., 2011), but the debate lacks a systematic study of how assumptions and uncertainties in the statistical models that describe element partitioning affect model outcomes. This makes it difficult to discern where the differences among physical model outcomes originate. Here we address two key questions relevant to evaluating equilibrium core formation models: (1) How do choices made during statistical modeling of the data, such as the form of the independent variables and the regression method, affect physical model outcomes? (2) Are the available experimental data precise enough to develop a unique physical model or discriminate between competing physical models?

We investigate these questions by close inspection of the statistical regression models of experimental data for four siderophile elements: Ni, Co, W, and V. We chose these elements because their mantle abundances are generally well-constrained, data sets of 20 or more experiments in the pressure range of ~ 5 –25 GPa are available for each element from a single laboratory, and as a group they provide good leverage on the variables of pressure, temperature, oxygen fugacity, and silicate melt composition. We only draw on a subset of the published data in order to avoid systematic biases that arise when combining data sets from multiple labs. We assess the statistical regression models that describe the experimental partitioning data to determine how tightly the regression models can constrain the variables of core formation, and to elucidate how those constraints depend on the chosen regression model.

2. Methodology

Partitioning experiments equilibrate metal and silicate over a range of pressures (P), temperatures (T), oxygen fugacities (fO_2), and metal and silicate compositions. In order to capture the variation of individual parameters, multivariable regression has been used extensively, both on individual data sets and in data compilations. To assess the impact of regression model and uncertainty on core formation modeling, we cull raw data from the literature, process it in a consistent manner, and regress the data using a variety of regression models. We then apply the regressions in models of core formation and take account of

the regression uncertainties using a Monte Carlo random-sampling technique.

2.1. Data

2.1.1. Selection of experimental data sets

We focus on four elements from three high-pressure data sets. Each data set was generated within a single laboratory ensuring a standard experimental and analytical approach, and thereby avoiding intra-element uncertainty derived from inter-laboratory bias. We use the Ni and Co data of Kegler et al. (2008), the V data of Wade and Wood (2001, 2005) and Wood et al. (2008), and the W data of Cottrell et al. (2009, 2010) (see Table A1 in Appendix A). Each data set has: (1) at least 22 experiments at ≥ 5 GPa (data at pressures less than 5 GPa are excluded to avoid non-linear effects of pressure indicated in the data sets of Kegler et al. (2008) and Cottrell et al. (2009) in the lower pressure regime), (2) a relatively large range in the variables P , T , composition, and oxygen fugacity, and (3) metal compositions to which we can apply the activity model of Wade and Wood (2005). The last point precludes the large and influential Ni and Co data set of Li and Agee (1996, 2001) because the metals in these experiments contain ~ 30 wt% S.

2.1.2. Activity models

The iron-rich metal solvents in partitioning experiments may contain a variety of solutes. Interactions among the solutes and solvent can lead to deviations from ideal solution behavior, such that the abundance of an element is not proportional to its activity. This is a potentially large source of inter-experiment bias if a variety of metal compositions are used or if the concentration of a solute changes as a function of P and T . Corrections to the measured abundances to values in pure iron metal at infinite dilution are possible if interaction parameters are known, in which case partition coefficients among different experiments can then be directly compared. Here, we employ the algorithm of Wade and Wood (2005) (<http://www.earth.ox.ac.uk/~expet/metal/>) to correct for solute–solute interactions in the iron alloy (see also Corgne et al. (2008)). This algorithm is based on interaction parameters and temperature extrapolations presented in the Steelmaking Data Sourcebook (Steelmaking, 1988) and the thermodynamic approach of Ma (2001). The inputs are the experimentally measured element mol fractions and run temperature, and the outputs are element activities at a given temperature.

Carbon is a solute in many of the experimental metals and can have large effects on partitioning (Cottrell et al., 2009). Due to analytical difficulties in measuring C accurately, the algorithm estimates the high temperature carbon content of all carbon-bearing metals on the basis of the free energy of dissolution at carbon saturation which is constrained by the experimentally determined 1 atm melt+graphite liquidus (Shunk, 1969). This is appropriate as all C-bearing experiments were made in graphite capsules and so metals should be C saturated.

2.1.3. The dependent variable

The dependent variable describes how each element (M) is distributed between the metal and silicate phases. For each experiment in this study, we calculated partition and distribution coefficients for each activity-corrected experiment as follows:

$$D_M = \frac{a_M^{\text{metal}}}{X_M^{\text{silicate}}} \quad (1)$$

$$K_D = \frac{(X_{\text{FeO}}^{\text{silicate}})^{n/2} (a_M^{\text{metal}})}{(a_{\text{MFe}}^{\text{metal}})(a_{\text{MO}_{n/2}}^{\text{metal}})} \quad (2)$$

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