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# PlanetBuilder 1.0: An open-source model to analyse the geochemical evolution of rocky planets during accretion and core formation

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**Abstract.** The chemical compositions of the silicate mantle and iron-rich metallic core of rocky planets are primarily determined by core formation during planetary accretion. For large planetary bodies, such as the Earth, accretion and core formation are complex, continuous processes that take place over millions of years, accompanied by increases in interior pressures and temperatures, changes in compositions and sizes of impactors and variations in the extent of core-mantle equilibration. PlanetBuilder is a new open-source Python-based geochemical multi-stage core formation program, designed to model these complex core formation processes. Using experimentally-derived metal-silicate element partitioning and mass-balance equations, the chemical equilibration between multiple series of (differentiated) impactors and the planetary body can be calculated to derive the bulk core and mantle compositions of continuously growing rocky planetary bodies. Our model combines methodologies from several established geochemical tools, and uses a thermodynamic oxygen partitioning model to verify if the metal-silicate equilibration is complete. PlanetBuilder is designed to handle different planetary and impactor compositions and conditions, as well as multiple elements simultaneously. Due to its reliance on oxygen partitioning, the model is not equipped to handle very oxidised impactors or volatile elements well. One of the main features of PlanetBuilder is the option to correct metal-silicate distribution for non-ideal behaviour of elements in metallic iron-rich liquids. Using a canonical Earth formation model as an example, we show that incorporating non-ideality can change predicted mantle element abundances after core formation by tens of percents, well outside the accuracy of terrestrial mantle abundance estimates. Due to our model's sensitivity to small changes in key parameters (e.g. equilibrium constants and exchange coefficients), it can be a valuable tool for reviewing a parameter's influence on predicted core and mantle compositions.

## 1 Introduction

Metallic core formation is a key process during the initial differentiation of rocky planetary bodies (e.g. Urey, 1951; Shaw, 1979; Trønnes et al., 2019). Accretionary and radiogenic heat, combined with the large density differences between the metallic and silicate/oxide phases that make up rocky planets, drive the physical process of separation and migration of molten metal to the centre of the planetary body, forming a metallic core surrounded by a partially to fully molten silicate-rich mantle. Metal segregation to a central core leaves a major chemical imprint on the composition of the outer silicate rock reservoir. Iron itself and other siderophile (iron-loving) elements are preferentially sequestered into core-forming metal, whereas lithophile (rock-loving) elements are enriched in the silicate part upon extraction of siderophiles. This imprint can be measured by analysing the

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major and trace element composition of surface and interior rock samples. Combining such analyses with models for the bulk composition of rocky planets enables us to produce core formation depletion patterns. Such patterns are available for Earth, Moon, Mars, and the asteroid Vesta – the only rocky bodies for which unambiguous samples of the silicate mantle and/or crust have been identified (Papike, 1998).

Geochemists use these patterns to constrain the conditions under which metal and silicate equilibrated during core formation. Understanding and simulating geochemical core formation therefore requires assessing metal-silicate partitioning processes, as partitioning and equilibration reactions can be used to calculate the chemical effects of metal segregation from the silicate mantle. Metal-silicate partitioning, the driving force behind the equilibration processes, is primarily studied through high-pressure-temperature experiments and geochemical modelling. Experimental studies typically aim to systematically quantify how variations in pressure ($P$), temperature ($T$), composition ($X$) and oxygen fugacity ($fO_2$) affect metal-silicate elemental partitioning (e.g. Hillgren et al., 1996; Rose-Weston et al., 2009; Siebert et al., 2011; Fischer et al., 2015). Most experimental studies focus on conditions and compositions that overlap with those of the interior of the Earth (e.g. Wade and Wood, 2005; Frost et al., 2010; Siebert et al., 2011; Righter et al., 2017), the Moon (e.g. Chabot and Agee, 2003; Rai and van Westrenen, 2014; Steenstra et al., 2016b), and to a lesser extent, other planetary bodies in our Solar System such as Mercury (e.g. Chabot et al., 2014; Namur et al., 2016; Cartier et al., 2024; Boujibar et al., 2024), Mars (e.g. Chi et al., 2014; Li et al., 2017; Righter et al., 2020; Gendre et al., 2022), and Vesta (e.g. Steenstra et al., 2016a). These studies provide parameterisations of metal-silicate partition coefficients (defined as the ratio in concentrations by weight of an element in metal and co-existing silicate) over a large pressure-temperature-composition ($PTX$) range (e.g. Siebert et al., 2011; Chabot et al., 2014; Steenstra et al., 2016a; Gendre et al., 2022). Such parametrisations are then used as input parameters for geochemical models of planetary core formation, together with physical models of the pressure and temperature conditions in a growing or fully accreted planet. A model is deemed successful if the modelled abundances of the elements considered in the silicate reservoir of a planet match the measured abundances in silicate samples. Although successful models are usually non-unique, they provide at least some constraints on the pressures and temperatures associated with core formation – constraints that remain very difficult to obtain through other means.

Geochemical core formation models aim to calculate the chemical compositions of the core and mantle of a planetary body during metal-silicate differentiation. In their simplest forms, so-called single-stage equilibration models, approximate chemical equilibration between the bulk planetary silicate reservoir (mantle and the later formed crust) and bulk planetary core as a single event at a particular pressure, temperature, composition, and oxygen fugacity (e.g. Corgne et al., 2008; Rubie et al., 2011; Chabot et al., 2014; Chidester et al., 2022). These models typically assume the presence of a global magma ocean throughout the accretion process to facilitate efficient molten metal - molten silicate equilibration. Therefore, single-stage equilibration models are especially useful in combination with metal-silicate experiments to provide insight into the element distribution in smaller planetary bodies and satellites such as the Moon and Vesta (e.g. Rai and van Westrenen, 2014; Steenstra et al., 2016a, 2017a).

Larger rocky planetary bodies, such as the Earth, have more complex accretion and core formation histories that took place over prolonged periods of time. These processes are best modelled through multi-stage core formation models, in which metal

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segregation is considered to be a continuous and dynamic process. During planetary accretion, multiple series of energetic impacts of large rocky bodies increase the mass of the planetary body and are accompanied by large-scale melting events. This results in the creation of deep magma oceans underlain by solid mantle material. In their simplest forms, multi-stage core formation models assess molten metal-molten silicate equilibration on the floor of a magma ocean, after which the liquid metal sinks through the solid lower mantle towards the centre of the planetary body without significant chemical interaction with solid silicates and oxides (e.g. Rubie et al., 2003; Wood et al., 2006; Fischer et al., 2015). As larger impactor cores require more time to emulsify and equilibrate completely with a surrounding magma ocean, their equilibration might be incomplete depending on the conditions within the magma ocean (e.g. Rubie et al., 2003; Dahl and Stevenson, 2010; Fischer et al., 2017; Landeau et al., 2021). Chemically this can result in (part of) larger impactor cores being transported to the core of a growing planet without chemical re-equilibration. Regardless of this degree of equilibration, the residual impactor cores are subsequently added to the planetary core. Contrary to single-stage core formation, the bulk planetary core is not in equilibrium with the bulk planetary mantle, as the metal-silicate equilibration occurs between the planetary mantle and the impactor core.

Here, we present PlanetBuilder, an open-source geochemical multi-stage core formation program that combines methodologies from existing geochemical models first described by Wade and Wood (2005) and Rubie et al. (2011). Our model calculates the chemical compositions for a continuously growing planetary mantle and core during accretion through metal-silicate partitioning and mass-balance calculations. We also include the option to correct the calculations by quantifying the non-ideal behaviour of elements in metallic iron-rich liquids during the metal-silicate equilibration process, using an implementation of the metallurgical model from Ma (2001).

PlanetBuilder is written in Python and follows a modular programming approach that allows individual sections to be easily modified and/or extended. As all parameterizations, conditions and compositions for both the growing planet and impactors can be adjusted, the model can be used for various types and sizes of rocky planetary bodies, both within and beyond our own solar system. In this paper, we present the functionality of our model, and discuss the possibilities, assumptions, and limitations. The fully annotated code, along with a manual, are included.

## 2 Model description

PlanetBuilder calculates the evolution of the chemical bulk compositions of a growing planetary mantle and planetary core through multi-stage core formation during accretion. The growth of the planetary body is represented as a series of discrete ‘accretion steps’ with impactors of known composition. Each impactor accreting to the planetary body marks the start of a new accretion step, during which metal-silicate equilibration processes, for all elements that the user wishes to consider, are completed. The accretion steps in the model do not include a timescale, and a timeframe for core formation is not set. A schematic overview of the model workflow for a single accretion step is presented in Fig. 1.

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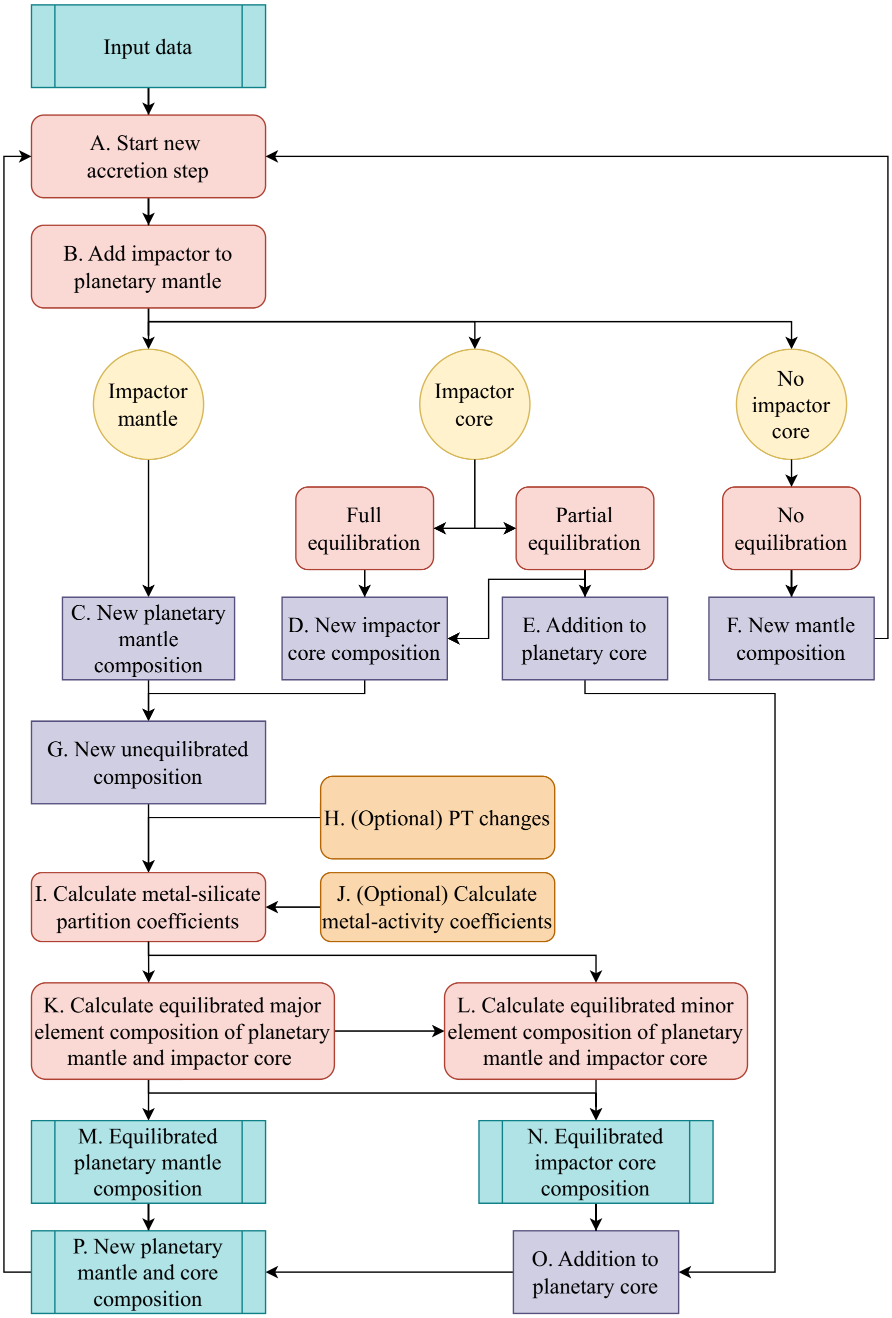


**Figure 1.** A schematic overview of PlanetBuilder. The input data at the top of the diagram includes the model settings, starting abundances of all elements considered in the planetary body, the composition and size of the impactor and the metal-silicate equilibration pressure-temperature conditions. The letters in front of the different steps are added for clarity, and to facilitate referencing in Sect. 2.

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Our model distinguishes between four compositionally different reservoirs: planetary mantle, planetary core, impactor mantle and impactor core. The planetary core is considered a semi-closed system: material is added through impactor cores, but it does not interact with the planetary mantle or the impactor mantle. All metal-silicate equilibration reactions occur between the planetary mantle (including impactor mantle material) and impactor core. Given the assumption that one or more deep magma oceans are present due to large-scale melting from energetic impacts, both the planetary mantle and impactor core are considered to be in a molten state, facilitating efficient metal-silicate equilibration.

When the impactor hits the planetary body at the start of a new accretion step (Fig. 1A, denoting step A in Fig. 1), the silicate-rich material of the impactor mantle is added to the bulk planetary mantle (Fig. 1B-C). If the impactor is so oxidised that it lacks a core, no metal-silicate equilibration occurs and the model continues to the next accretion step (Fig. 1F). If the impactor has a core, the dense metal liquid is expected to sink through the magma ocean towards the magma ocean floor, and eventually onwards through the solid lower parts of the mantle to the centre of the planetary body. During its descent through the magma ocean and while residing on the magma ocean floor, the metal liquid (partially) equilibrates with the molten silicate mantle. Partial equilibration is modelled by splitting the impactor core into two parts: one part is available for metal-silicate equilibration (Fig. 1D) and the other part is excluded from metal-silicate equilibration and is directly added to the planetary core (Fig. 1E). The resulting unequilibrated compositions of the planetary mantle (Fig. 1C) and impactor core (Fig. 1D) are considered as the starting input for metal-silicate equilibration calculations (Fig. 1G). Based on user-defined pressure-temperature conditions and optional changes for the given accretion step (Fig. 1H), the equilibrium impactor core – planetary mantle partitioning of all elements considered is calculated (Fig. 1I). These calculations are explained in more detail in Sect. 2.1 - 2.3. More information on the optional incorporation of corrections for the non-ideal activity relations of elements in the metal liquid (Fig. 1J) and its influence on metal-silicate partitioning is provided in Sect. 2.4.

Central to PlanetBuilder are metal-silicate partitioning parametrisations (Sect. 2.1) and mass balance calculations (Sect. 2.2), based on the methodology outlined in Rubie et al. (2011). Whereas metal-silicate partitioning parametrisations describe the distribution of elements between molten metal and molten silicate, the corresponding mass balance equations ensure that the total abundance of elements in the planetary mantle and impactor core combined remains constant. Through these calculations, the chemical compositions of the (partially) equilibrated impactor core and planetary mantle can be determined. First, the major element compositions of the equilibrated planetary mantle and impactor core are determined (Fig. 1K), as detailed in Sect. 2.3. The equilibrated major element compositions and metal-silicate partitioning equations (which can include assessments of non-ideal behaviour in the metal as described in Sect. 2.4) are then used to derive the accompanying minor and trace element distributions between the planetary mantle and impactor core in Sect. 2.5 (Fig. 1L). The resulting equilibrated planetary mantle composition (Fig. 1M) is used as the new composition of the planetary mantle at the start of the next accretion step (Fig. 1P). The equilibrated impactor core (Fig. 1N) is added to the planetary core (Fig. 1O), which serves as the planetary core composition at the start of the next accretion step (Fig. 1P).

Although in reality the conditions for equilibration between the impactor core and planetary mantle are changing continuously as the metal liquid sinks through the magma ocean, it is not feasible to model the interactions over a range of increasing pressures and temperatures associated with an increase in depth. Therefore, every impact is associated with a so-called ef-

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fective pressure and effective temperature thought to provide reasonable estimates for the average conditions at which the metal-silicate equilibration reactions occur. Estimates for the effective pressure and temperature are commonly assumed to reflect conditions at the bottom of the magma ocean, where most of the equilibration is expected to occur (e.g. Rubie et al., 2003; Wade and Wood, 2005; Kegler et al., 2008; Righter, 2015). Several studies suggest this is due to a layer of liquid metal ponding at the bottom of the magma ocean, whereas other studies suggest that small metal droplets equilibrate near the bottom of the magma ocean (Stevenson, 1990; Rubie et al., 2003; Sasaki and Abe, 2007). The magma ocean is separated from the planetary core by an underlying layer of high-viscosity solid silicate mantle, preventing direct transfer of the metal liquid from the magma ocean to the planetary core, and preventing direct equilibration between the planetary mantle and planetary core. As the metal liquid at the bottom of the magma ocean is denser than the underlying solid silicate mantle, once a sufficient volume of metal is collected at the magma ocean bottom, a 'negative diapir' is commonly thought to form, upon which the metal liquid quickly descends further towards the planetary core (e.g. Wood et al., 2006; Samuel and Tackley, 2008). Although this transport mechanism remains subject of debate, it is not considered to be part of our model, as we focus purely on the chemical result where metal liquid is added to the planetary core (e.g. Stevenson, 1990; Samuel and Tackley, 2008; Lherm and Deguen, 2018).

## 2.1 Metal-silicate partitioning

The metal-silicate partitioning behaviour of an element M determines the distribution of M between the liquid impactor core (metal) and the molten planetary mantle (silicate) during equilibration. The distribution is determined by the thermodynamics of a reduction-oxidation (redox) reaction between the reduced metal core and oxidised silicate mantle:

$$\mathrm{M}^{\mathrm{metal}} + \frac{\mathrm{n}}{4}\mathrm{O}_2 = \mathrm{MO}_{\mathrm{n}/2}^{\mathrm{silicate}} \tag{1}$$

where n is the valence of element M (e.g. Wade and Wood, 2005; Siebert et al., 2011). The ratio between the concentrations of M in metal and silicate phase at equilibrium is described by the partitioning coefficient $\mathrm{D_M}$:

$$\mathrm{D_M} = \frac{\mathrm{x}_{\mathrm{M}}^{\mathrm{metal}}}{\mathrm{x}_{\mathrm{MO}_{\mathrm{n}/2}}^{\mathrm{silicate}}} \tag{2}$$

where x is the molar fraction of element M and its corresponding oxide in respective phases (e.g. Righter, 2003; Wade and Wood, 2005; Siebert et al., 2011). Experimental metal-silicate partitioning studies show that partition coefficients ($\mathrm{D_M}$) can be strongly affected by changes in pressure ($P$), temperature ($T$), oxygen fugacity ($f\mathrm{O}_2$) and melt composition, even though this is not reflected in their definitions (Eq. 1).

The oxygen fugacity ($f\mathrm{O}_2$) is a thermodynamic property that is used to describe the oxidation state of the overall planet (Eq. 1). Although oxygen fugacity plays an important role in metal-silicate partitioning, precisely determining its effect remains difficult due to its sensitivity to changes in pressure and temperature as well as non-ideal gas behaviour. A commonly used approximation for the oxygen fugacity is to express it in terms of the oxidation state of iron (e.g. Wade and Wood, 2005; Corgne et al., 2008). Fe and FeO are two major components of the planetary core and mantle, respectively, and directly related

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to changes in the oxygen fugacity through the chemical reaction:

$$2\mathrm{Fe} + \mathrm{O_2} = \mathrm{FeO} \tag{3}$$

The oxygen fugacity is often expressed relative to the oxygen fugacity of the iron-wüstite buffer, which is defined by the equilibrium of metallic iron (Fe) and iron oxide (FeO) and based on the chemical reaction of Eq. (3) (e.g. Drake et al., 1989). The oxygen fugacity relative to this iron-wüstite equilibrium ($\Delta$IW) is given by:

$$\Delta\mathrm{IW} = 2\log\left(\frac{\mathrm{a_{FeO}^{silicate}}}{\mathrm{a_{Fe}^{metal}}}\right) \tag{4}$$

where $\mathrm{a}$ is the activity of FeO and Fe in the silicate melt and molten metal, respectively. The activity is a thermodynamic property that describes the effective concentrations of FeO and Fe in the silicate and metal (e.g. Drake et al., 1989). It can be calculated from the activity coefficient ($\gamma$) and mole fraction (x) and implemented into Eq. (4) to yield:

$$\Delta\mathrm{IW} = 2\log\left(\frac{\mathrm{x_{FeO}^{silicate}}}{\mathrm{x_{Fe}^{metal}}}\right) + 2\log\left(\frac{\gamma_{\mathrm{FeO}}^{\mathrm{silicate}}}{\gamma_{\mathrm{Fe}}^{\mathrm{metal}}}\right) \tag{5}$$

The activity coefficient ($\gamma$) is a correction factor for non-ideal mixing behaviour due to interactions with other elements present. Therefore, the activity coefficient and oxygen fugacity are directly related to compositional changes within the core and mantle. To include the effect of Fe and FeO, the exchange reaction of Eq. (1) can be combined with Eq. (3):

$$\mathrm{MO_{n/2}^{silicate}} + \frac{\mathrm{n}}{2}\mathrm{Fe^{metal}} = \frac{\mathrm{n}}{2}\mathrm{FeO^{silicate}} + \mathrm{M^{metal}} \tag{6}$$

The corresponding exchange coefficient $\mathrm{K_M^D}$, which is dependent on the mole fractions of Fe and element M in both metal and silicate, is then described as:

$$\mathrm{K_M^D} = \frac{\mathrm{x_M^{metal}}(\mathrm{x_{FeO}^{silicate}})^{\mathrm{n}/2}}{\mathrm{x_{MO_{n/2}}^{silicate}}(\mathrm{x_{Fe}^{metal}})^{\mathrm{n}/2}} \tag{7}$$

Expanding Eq. (7) to include the activity coefficients as described in Eq. (5) gives the equilibrium constant $\mathrm{K_M^A}$:

$$\log\mathrm{K_M^A} = \log\underbrace{\frac{(\mathrm{x_{FeO}^{silicate}})^{\mathrm{n}/2}\cdot(\mathrm{x_M^{metal}})}{(\mathrm{x_{MO_{n/2}}^{silicate}})\cdot(\mathrm{x_{Fe}^{metal}})^{\mathrm{n}/2}}}_{\mathrm{K_M^D}} + \log\frac{\gamma_{\mathrm{M}}^{\mathrm{metal}}}{(\gamma_{\mathrm{Fe}}^{\mathrm{metal}})^{\mathrm{n}/2}} + \log\frac{(\gamma_{\mathrm{FeO}}^{\mathrm{silicate}})^{\mathrm{n}/2}}{(\gamma_{\mathrm{MO_{n/2}}}^{\mathrm{silicate}})} \tag{8}$$

Previous studies indicate that the oxide activity coefficients - gathered in the last term on the right hand side of Eq.(8) - are not strongly affected by changes in the silicate melt composition (e.g. Holzheid et al., 1997; O'Neill and Eggins, 2002; Wade and Wood, 2005). The experimental partitioning data for $\mathrm{SiO_2}$, NiO and CoO indicate an activity behaviour in the silicate melt similar to that of FeO. Therefore, the ratios of the oxide activity coefficients are assumed to be constant, simplifying Eq. (8) to calculate the apparent equilibrium constant $\mathrm{K_M^{App}}$:

$$\log\mathrm{K_M^{App}} = \log\mathrm{K_M^D} + \log\frac{(\gamma_{\mathrm{M}}^{\mathrm{metal}})}{(\gamma_{\mathrm{Fe}}^{\mathrm{metal}})^{\mathrm{n}/2}} \tag{9}$$

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Many commonly used multi-stage core formation models still assume ideal mixing behaviour in metals with all $\gamma$ values set equal to 1, which makes the final term in Eq. (9) equal to zero and $\mathrm{K_M^{App}}$ equal to $\mathrm{K_M^D}$ (Eq. 7) (e.g. Rubie et al., 2011, 2015; Fischer et al., 2017). This simplifying assumption can also be applied in PlanetBuilder. However, contrary to the activity of elements in silicate melts, the activity of elements in molten metal known to be affected significantly by changes in metal compositions (e.g. Wade and Wood, 2005; Corgne et al., 2008; Tuff et al., 2011; Steenstra et al., 2017b; Jennings et al., 2021). Therefore, corrections to account for the effect that changes in metal activity have on $\mathrm{K_M^{App}}$ and $\mathrm{K_M^D}$ can be important for the chemical modelling of core formation.

Activity correction values are often based on data gathered at atmospheric pressure from the steelmaking industry and are then extrapolated to higher *PT* conditions (e.g. The Japan Society for the Promotion of Science, 1988; Wade and Wood, 2005; Corgne et al., 2008). The assumptions that were made to extrapolate data to an unexplored range of *PT* conditions could result in large errors and inaccurate correction values. Several recent experimental studies show that high-pressure activity coefficients obtained directly from experiments are not the same as those predicted by low-pressure steelmaking data (e.g. Steenstra et al., 2017b; Righter et al., 2020). This difference leaves room for discussion on the accuracy of the metal activity coefficients. In this study we do not weigh in on the discussion. However, one of the important features of our model is the option to incorporate and quantitatively assess the effect of using both classic (steelmaking-derived) and new metal activity coefficients, compared to the simplifying assumption assuming metal ideality that is used in many other core formation applications. This is further explained in Sect. 2.4 and Sect. 3.2.

In PlanetBuilder, the effective equilibration pressure and temperature at a given accretion step remain constant throughout the equilibration process. Their effect on the distribution of element M can be parametrised as:

$$\log \mathrm{K_M^{App}} = \mathrm{a} + \frac{\mathrm{b}}{\mathrm{T}} + \frac{\mathrm{cP}}{\mathrm{T}} \tag{10}$$

where *T* and *P* are the temperature in K and pressure in GPa, respectively. The regression coefficients a, b and c are constants determined by fitting Eq. (10) to a large set of experimentally derived $\mathrm{K_M^{App}}$ values, ideally covering the full pressure and temperature range to be considered in a particular model. PlanetBuilder incorporates an initial set of parameterisations for eight major and trace elements taken from a variety of literature sources, with values for the fit parameters a, b and c and associated uncertainties shown in Table 1.

If the planetary mantle and impactor core are in equilibrium, the equilibrium constant based on *PT* conditions in Eq. (10) should be equal to the equilibrium constant based on the melt compositions corrected for activity behaviour (Eq. 9):

$$\log \mathrm{K_M^D} + \log \frac{(\gamma_\mathrm{M}^\mathrm{met})}{(\gamma_\mathrm{Fe}^\mathrm{met})^{\mathrm{n}/2}} = \mathrm{a} + \frac{\mathrm{b}}{\mathrm{T}} + \frac{\mathrm{cP}}{\mathrm{T}} \tag{11}$$

As the *PT* conditions are kept constant during metal-silicate equilibration in our model, the right-hand side of Eq. (11) can be treated as a constant. Therefore, the left-hand side of the Eq. (11) can be used to derive equilibrated compositions for the planetary mantle and impactor core. The complexity of this derivation depends on the inclusion of activity corrections, as explained further in Sect. 2.4.

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**Table 1.** Parameterisations for regression coefficients

| Element | N | a | b | c | Source |
|---|---|---|---|---|---|
| Ni | $2^+$ | $0.46 \pm 0.16$ | $2700 \pm 300$ | $-61 \pm 6$ | Fischer et al. (2015) |
| Si | $4^+$ | $1.3 \pm 0.3$ | $-13500 \pm 900$ | | Fischer et al. (2015) |
| Co | $2^+$ | $0.36 \pm 0.15$ | $1500 \pm 300$ | $-33 \pm 5$ | Fischer et al. (2015) |
| Cr | $2^+$ | $0.0 \pm 0.3$ | $2900 \pm 700$ | $9 \pm 11$ | Fischer et al. (2015) |
| Nb | $5^+$ | $2.66 \pm 0.11$ | $-14032$ | $-199 \pm 16$ | Mann et al. (2009) |
| Ta | $5^+$ | $0.84 \pm 0.09$ | $-13806$ | $-101 \pm 15$ | Mann et al. (2009) |
| V | $3^+$ | $-0.3 \pm 0.6$ | $-5400 \pm 1200$ | $19 \pm 19$ | Fischer et al. (2015) |
| W | $4.4^+$ | $-0.35 \pm 0.46$ | $1209 \pm 1005$ | $-114 \pm 13$ | Cottrell et al. (2009, 2010) |

Values for a, b and c as used in Eq. (10). Uncertainties represent $1\sigma$

### 2.2 Mass balance

Mass balance equations are used in addition to metal-silicate partitioning calculations to ensure no material is lost when determining the equilibrated compositions. These reactions dictate that the mass of the initial unequilibrated liquids (metal and silicate) are equal to the mass of the final equilibrated liquids (metal and silicate). The mass balance equations for individual elements are intrinsically coupled, as cations in the silicate mantle typically occur as oxides, linking their individual mass balance equations to that of oxygen. Therefore, the model is required to solve all mass-balance equations simultaneously, which increases complexity as more elements are considered. We used a similar approach to that of Rubie et al. (2011), focusing on the partitioning of major elements Fe, Si, Ni and O and using these results to determine the metal-silicate partitioning behaviour of any other minor or trace element. For Earth-like compositions, Mg, Al and Ca are expected to be key components of the bulk silicate mantle. As these are all highly lithophile and refractory elements, they are not thought to dissolve substantially in liquid Fe nor to actively participate in metal-silicate equilibration under most conditions (e.g. McDonough and Sun, 1995; Helffrich et al., 2020; Chidester et al., 2022). Therefore, Mg, Al and Ca are assumed to remain in the silicate mantle throughout the accretion process as oxide components MgO, $Al_2O_3$ and CaO, respectively (e.g. Wade and Wood, 2005; Rubie et al., 2011). The major element mass-balance calculation that is initially solved by the model can therefore be simplified to:

$$(\mathrm{FeO} + \mathrm{NiO} + \mathrm{SiO_2})_{\mathrm{old}} + (\mathrm{Fe} + \mathrm{Ni} + \mathrm{Si} + \mathrm{O})_{\mathrm{old}} = (\mathrm{FeO} + \mathrm{NiO} + \mathrm{SiO_2})_{\mathrm{new}} + (\mathrm{Fe} + \mathrm{Ni} + \mathrm{Si} + \mathrm{O})_{\mathrm{new}} \quad (12)$$

where the concentrations of all components are expressed in moles. The old and new in these equations refers to the unequilibrated and equilibrated compositions, respectively. The individual mass balance equations which are simultaneously solved

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can be written as:

$$\mathrm{Fe}: \mathrm{FeO}_{\mathrm{old}} + \mathrm{Fe}_{\mathrm{old}} = \mathrm{FeO}_{\mathrm{new}} + \mathrm{Fe}_{\mathrm{new}} \tag{13}$$

$$\mathrm{Si}: \mathrm{SiO}_{2\,\mathrm{old}} + \mathrm{Si}_{\mathrm{old}} = \mathrm{SiO}_{2\,\mathrm{new}} + \mathrm{Si}_{\mathrm{new}} \tag{14}$$

$$\mathrm{Ni}: \mathrm{NiO}_{\mathrm{old}} + \mathrm{Ni}_{\mathrm{old}} = \mathrm{NiO}_{\mathrm{new}} + \mathrm{Ni}_{\mathrm{new}} \tag{15}$$

$$\mathrm{O}: \mathrm{FeO}_{\mathrm{old}} + 2\mathrm{SiO}_{2\,\mathrm{old}} + \mathrm{NiO}_{\mathrm{old}} + \mathrm{O}_{\mathrm{old}} = \mathrm{FeO}_{\mathrm{new}} + 2\mathrm{SiO}_{2\,\mathrm{new}} + \mathrm{NiO}_{\mathrm{new}} + \mathrm{O}_{\mathrm{new}} \tag{16}$$

### 2.3 Solving the metal-silicate partitioning behaviour of Fe, Si, Ni and O

Determining the Fe, Si, Ni and O concentrations of the equilibrated metal impactor core and planetary silicate mantle requires the application of a complex solver, as multiple variables must be balanced while their partitioning behaviour is not linear. The seven unknown variables to solve simultaneously are the $\mathrm{FeO}$, $\mathrm{SiO_2}$ and $\mathrm{NiO}$ abundances in the planetary mantle and the Fe, Si, Ni and O abundances of the equilibrating impactor core. We opted to use the Mixed Integer Distributed Ant Colony Optimization (MIDACO) solver (Schlueter et al., 2013), due to its efficiency and accuracy. Our published code therefore includes a limited version of MIDACO, licensed under CC BY-NC-ND (Schlueter et al., 2013). Every iteration of the solver follows the same procedure, where a set of new values for the unknown variables is derived and tested. A schematic overview of the procedure and calculations within the solver is shown in Fig. 2. The first part of the procedure (Fig. 2B to Fig. 2G, and Sect. 2.3.1) is used to calculate hypothetical equilibrated major element compositions for the planetary mantle and impactor core. The solver selects a value for the new $\mathrm{FeO}$ abundance of the planetary mantle, which is used to derive all other corresponding abundances in both planetary mantle and impactor core based on mass-balance and metal-silicate partitioning equations. The second part of the procedure (Fig. 2H to Fig. 2K and Sect. 2.3.2) is used to test if this hypothetical composition is in equilibration by comparing the $\mathrm{K_O^D}$ of the composition with the thermodynamically calculated $\mathrm{K_O^D}$ of Frost et al. (2010). A valid solution requires the difference between the two $\mathrm{K_O^D}$ values to be smaller than the uncertainty (default: $< 10^{-4}$). If there is no convergence, the $\mathrm{FeO}$ concentration in the planetary mantle is adjusted and the process repeated (Fig. 2L). Once solved, the program checks whether any (more) corrections are needed for the activity of elements in molten metal (Fig. 2M). These corrections and their influence on the workflow of the solver (Fig. 2N) are explained in Sect. 2.4.

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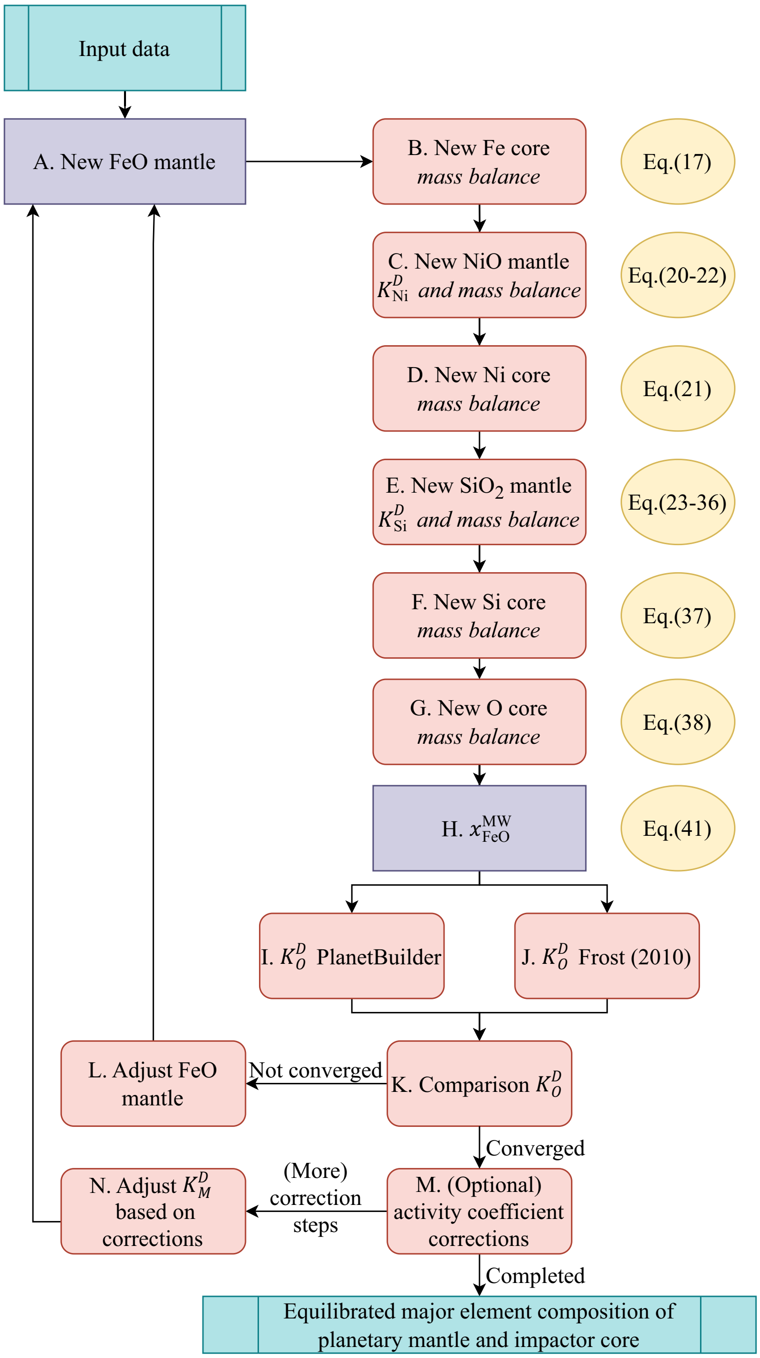


**Figure 2.** A schematic overview of the procedure and equations that are used inside the MIDACO solver. The input data at the top of the diagram includes the unequilibrated compositions of the planetary mantle and impactor core, along with the exchange and equilibration coefficients. Similar to Fig. 1, the letters in front of the different steps are used to facilitate referencing in Sect. 2.3.

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#### 2.3.1 Calculating hypothetical compositions for the planetary mantle and impactor core

The input for the solver contains the unequilibrated compositions of the planetary mantle and impactor core. The $K_M^D$ values for Si and Ni are dependent on pressure and temperature and do not change throughout the accretion step. To reduce computation time, $K_{Si}^D$ and $K_{Ni}^D$ are calculated beforehand, as part of the solver input, from Eq. (10), using parameters from Table 1. At the start of every solver iteration a new value for $FeO_{new}$ is estimated (Fig. 2B). This functions as the starting point for calculating the other 6 unknowns and therefore the hypothetical equilibrated composition. The first iteration of the solver uses the $FeO_{old}$ from the input data (Fig. 2A). In every subsequent iteration the solver systematically alters the FeO value to approach a convergent solution. A new value for Fe ($Fe_{new}$) can be determined with $FeO_{new}$ and by mass-balance Eq. (14) (Fig. 2B):

$$\mathrm{Fe_{new}} = \mathrm{FeO_{old}} + \mathrm{Fe_{old}} - \mathrm{FeO_{new}} \tag{17}$$

From $Fe_{new}$ and $FeO_{new}$, the new abundances of the other major elements (Ni, NiO, Si, $SiO_2$) can be calculated. For elements with a valence state of $2^+$, the exchange coefficient $K_M^D$ in Eq. (7) and mass balance equation Eq. (12) can be used to express the major element composition in moles rather than molar fractions:

$$K_M^D = \frac{\frac{M^{metal}}{core} \cdot \frac{FeO^{silicate}}{mantle}}{\frac{MO^{silicate}}{mantle} \cdot \frac{Fe^{met}}{core}} = \frac{\frac{M^{metal}}{Fe+Si+Ni+O} \cdot \frac{FeO^{silicate}}{FeO+SiO_2+NiO+L}}{\frac{MO^{silicate}}{FeO+SiO_2+NiO+L} \cdot \frac{Fe^{metal}}{Fe+Si+Ni+O}} \tag{18}$$

where L is the sum of the total moles of refractory oxide components MgO, $Al_2O_3$ and CaO. This equation can be shortened to:

$$K_M^D = \frac{M^{metal} \cdot FeO}{MO^{silicate} \cdot Fe} \tag{19}$$

The new NiO concentration in the mantle ($NiO_{new}$) can be determined by combining Eq. (19) with the known values for the equilibrated Fe and FeO, along with the $K_{Ni}^D$ (Fig. 2C):

$$\mathrm{NiO_{new}} = \frac{\mathrm{FeO_{new}} \cdot \mathrm{Ni_{new}}}{\mathrm{Fe_{new}} \cdot K_{Ni}^D} \text{with} \tag{20}$$

$$\mathrm{Ni_{new}} = \mathrm{NiO_{old}} + \mathrm{Ni_{old}} + \mathrm{NiO_{new}} \tag{21}$$

Combining and simplifying these equations gives:

$$\mathrm{NiO_{new}} = \frac{\mathrm{FeO_{new}} \cdot (\mathrm{NiO_{old}} + \mathrm{Ni_{old}})}{\mathrm{Fe_{new}} \cdot K_{Ni}^D + \mathrm{FeO_{new}}} \tag{22}$$

With this new NiO concentration, the new concentration for Ni can also be calculated using the mass-balance as described in Eq.(21) for Fig. 2D. Determining the new $SiO_2$ values is more complex due to the $4^+$ valence state of Si. The redox equation of Eq. (1) then becomes:

$$\mathrm{SiO_2} + 2\mathrm{Fe} = \mathrm{Si} + 2\mathrm{FeO} \tag{23}$$

Therefore, the $K_M^D$ formula in Eq. (18) changes to:

$$K_{Si}^D = \frac{\frac{Si}{core} \cdot \left(\frac{FeO}{mantle}\right)^2}{\frac{SiO_2}{mantle} \cdot \left(\frac{Fe}{core}\right)^2} = \frac{Si \cdot FeO^2 \cdot core}{SiO_2 \cdot Fe^2 \cdot mantle} \tag{24}$$

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To calculate $SiO_{2\,new}$ (Fig. 2E), this equation can be modified to:

$$SiO_{2\,new} = \frac{Si_{new} \cdot FeO^2_{new} \cdot core}{x \cdot Fe^2_{new} \cdot mantle} - K^D_{Si} = 0 \tag{25}$$

Following the mass balance equations (Eq. 13-16), all unknown values from the mantle and core can be expressed in terms of $SiO_{2\,new}$. In the subsequent equations, $SiO_{2\,new}$ is shortened to the unknown variable x for readability :

$$Si_{new} = A - x \text{ with } A = SiO_{2\,old} + Si_{old} \tag{26}$$

$$O_{new} : B - 2x \text{ with } B = FeO_{old} + NiO_{old} + 2SiO_{2\,old} + O - FeO_{new} - NiO_{new} \tag{27}$$

$$core = Fe_{new} + Si_{new} + Ni_{new} + O_{new} = A - x + B - 2x + C \text{ with } C = Fe_{new} + Ni_{new} \tag{28}$$

$$mantle = FeO_{new} + x + NiO_{new} + L_{new} = D + x \text{ with } D = FeO_{new} + NiO_{new} + L_{new} \tag{29}$$

Substitution into Eq. (25) gives:

$$\frac{FeO^2_{new} \cdot (A - x)(A + B + C - 3x)}{Fe^2_{new} \cdot x(D + x)} - K^D_{Si} = 0 \tag{30}$$

Dividing this equation by $Fe^2_{new} \cdot x(D + x)$ and rewriting it gives:

$$FeO^2_{new} \cdot (A - x)(E - 3x) - K^D_{Si}(Fe^2_{new} \cdot x(D + x)) = 0 \text{ with } E = A + B + C \tag{31}$$

Expanding the factors gives:

$$FeO^2_{new} \cdot (A \cdot E - 3A \cdot x - E \cdot x + 3x^2) - K^D_{Si}(D \cdot Fe^2_{new} \cdot x + Fe^2_{new} \cdot x^2) = 0 \tag{32}$$

$$FeO^2_{new} \cdot 3x^2 - K^D_{Si} \cdot Fe^2_{new} \cdot x^2 - 3FeO^2_{new} \cdot A \cdot x - FeO^2_{new} \cdot E \cdot x - K^D_{Si} \cdot Fe^2_{new} \cdot D \cdot x + FeO^2_{new} \cdot A \cdot E = 0 \tag{33}$$

(34)

This equation can be written and solved as a quadric equation to find the value of $SiO_{2\,new}$ (x):

$$(3FeO^2_{new} - K^D_{Si} \cdot Fe^2_{new})x^2 - (3FeO^2_{new} \cdot A + FeO^2_{new} \cdot E + K^D_{Si} \cdot Fe^2_{new} \cdot D)x + FeO^2_{new} \cdot A \cdot E = 0 \tag{35}$$

$$SiO_{2\,new} = x = \frac{-b \pm \sqrt{b^2 - 4 \cdot a \cdot c}}{2 \cdot a} \text{ with: } a = 3 \cdot FeO^2_{new} \tag{36}$$

$$b = 3 \cdot FeO^2_{new} \cdot A + FeO^2_{new} \cdot E + K^D_{Si} \cdot Fe^2_{new} \cdot D$$

$$c = FeO^2_{new} \cdot A \cdot E$$

From the new $SiO_2$ concentration (Fig. 2E), the new Si abundance of the impactor core can be calculated by rearranging the mass-balance of Eq. (14) (Fig. 2F):

$$Si_{new} = SiO_{2\,old} + Si_{old} - SiO_{2\,new} \tag{37}$$

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From the partitioning of Fe, Si and Ni, the new abundance of oxygen in the impactor core can be calculated (Fig. 2G). In the planetary mantle, oxygen is primarily present in the form of oxides. Although major lithophile elements such as $\mathrm{MgO}$, $\mathrm{Al_2O_3}$ and $\mathrm{CaO}$ contain significant concentrations of oxygen, they do not actively participate in the metal-silicate equilibration and are therefore not considered for the mass-balance of oxygen (Sect. 2.2). Following Eq. (12), the relevant oxygen content for the planetary mantle can be derived from the abundances of $\mathrm{FeO}$, $\mathrm{NiO}$ and $\mathrm{SiO_2}$. The new concentration of oxygen in the impactor core is determined by rewriting mass-balance equation Eq. (16):

$$\mathrm{O_{new} = FeO_{old} + NiO_{old} + 2SiO_{2\,old} + O_{old} - FeO_{new} - NiO_{new} - 2SiO_{2\,new}} \tag{38}$$

### 2.3.2 Determining if the hypothetical compositions are in equilibrium

To determine if the compositions for the planetary mantle and impactor core as calculated in the first part of the solver are in equilibrium with each other, the exchange coefficient of O is derived in two different ways: (1) $\mathrm{K_O^D(PlanetBuilder)}$ is based on the metal-silicate partitioning of O in the hypothetical compositions of the planetary mantle and impactor core as calculated in PlanetBuilder using Eq. (38). (2) $\mathrm{K_O^D(Frost)}$ is based on the thermodynamic O partitioning model in the Fe-Mg-O system from Frost et al. (2010), which is based on experimental data obtained up to 70GPa and 3500K.

The exchange coefficient $\mathrm{K_M^D}$ as written in Eq. (7) cannot be used to describe the metal-silicate partitioning of oxygen, as it is directly related to the oxygen fugacity ($f\mathrm{O_2}$). Magnesiowüstite (MW) is often used as a proxy for silicate liquids in experimental studies on the partitioning of oxygen (e.g. Rubie et al., 2004; Asahara et al., 2007). The chemical reaction between Fe-rich metallic liquid and magnesiowüstite (MW) and corresponding exchange coefficient of oxygen can be described by (Asahara et al., 2007; Frost and McCammon, 2008):

$$\underset{\text{magnesiowüstite(MW)}}{\mathrm{FeO}} = \underset{\text{metal liquid}}{\mathrm{Fe+O}} \tag{39}$$

$$\mathrm{K_O^D} = \left(\frac{\mathrm{x_{Fe}^{metal} \cdot x_O^{metal}}}{\mathrm{x_{FeO}^{MW}}}\right) \tag{40}$$

Rubie et al. (2004) derived an empirical relationship between the FeO concentration of silicate liquid and magnesiowüstite, that can be used to relate the hypothetical silicate mantle to magnesiowüstite (Fig. 2H):

$$\mathrm{x_{FeO}^{MW}} = 1.148\mathrm{x_{FeO}^{silicate}} + 1.319(\mathrm{x_{FeO}^{silicate}})^2 \tag{41}$$

Although ideally the full set of core and mantle abundances of minor and trace elements would also be considered when determining the compositions of the planetary mantle or impactor core, their low total abundances have negligible influence on the equilibration of the major elements. The molar fractions of $\mathrm{FeO}$ in the planetary mantle and $\mathrm{Fe}$ and $\mathrm{O}$ in the impactor core

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from Eq. (40) are therefore inferred from the major elements of the respective phases used in the solver:

$$x_{\mathrm{FeO}}^{\mathrm{silicate}} = \frac{\mathrm{FeO_{new}}}{\mathrm{FeO_{new}} + \mathrm{NiO_{new}} + \mathrm{SiO_{2\,new}} + (\mathrm{MgO} + \mathrm{CaO} + \mathrm{Al_2O_3})_{\mathrm{new}}} \tag{42}$$

$$x_{\mathrm{Fe}}^{\mathrm{metal}} = \frac{\mathrm{Fe_{new}}}{\mathrm{Fe_{new}} + \mathrm{Si_{new}} + \mathrm{Ni_{new}} + \mathrm{O_{new}}} \tag{43}$$

$$x_{\mathrm{O}}^{\mathrm{metal}} = \frac{\mathrm{O_{new}}}{\mathrm{Fe_{new}} + \mathrm{Si_{new}} + \mathrm{Ni_{new}} + \mathrm{O_{new}}} \tag{44}$$

$$\tag{45}$$

The $K_O^D$ (PlanetBuilder) is derived from Eq. (40), whereas the thermodynamic description of $K_O^D$ (Frost) is described in Frost et al. (2010). Following Eq. (3-5) from Frost et al. (2010), the chemical potential of the impactor core and planetary mantle should be equal during equilibrium between the two phases.

$\mu_{\mathrm{FeO}}^{\mathrm{metal}} = \mu_{\mathrm{FeO}}^{\mathrm{MW}}$ with:

$$\begin{aligned} \mu_{\mathrm{FeO}}^{\mathrm{metal}} &= \mu_{\mathrm{FeO,P,T}}^{0,\mathrm{metal}} + \mathrm{RTln}(x_{\mathrm{FeO}}^{\mathrm{metal}}) + \mathrm{RTln}(\gamma_{\mathrm{FeO}}^{\mathrm{metal}}) \\ \mu_{\mathrm{FeO}}^{\mathrm{MW}} &= \mu_{\mathrm{FeO,P,T}}^{0,\mathrm{MW}} + \mathrm{RTln}(x_{\mathrm{FeO}}^{\mathrm{MW}}) + \mathrm{RTln}(\gamma_{\mathrm{FeO}}^{\mathrm{MW}}) \end{aligned} \tag{46}$$

where $\mu_{\mathrm{FeO,P,T}}^0$ is the standard state chemical potential, determined using the thermodynamic data from Frost et al. (2010), R is the gas constant, $x_{\mathrm{FeO}}$ and $\gamma_{\mathrm{FeO}}$ are the concentration and activity of FeO in either metal or magnesiowüstite. The last term of Eq. (46) can be derived from asymmetric Margules equations as described in Frost et al. (2010), which are also dependant on the concentration of FeO in metal and magnesiowüstite. While the $x_{\mathrm{FeO}}^{\mathrm{MW}}$ is calculated in Eq. (41), finding a $x_{\mathrm{FeO}}^{\mathrm{metal}}$ that results in the same chemical potential (Eq. 46) is more complex. With the $x_{\mathrm{FeO}}^{\mathrm{MW}}$ from the hypothetical composition as input, we use a second, smaller version of the MIDACO solver to efficiently find the $x_{\mathrm{FeO}}^{\mathrm{metal}}$, which tends to be $< 0.01\%$. This $x_{\mathrm{FeO}}^{\mathrm{metal}}$ value is then used to calculate a thermodynamically consistent $K_O^D$ (Frost et al., 2010; Rubie et al., 2011, 2015). These two derivations are described as Fig. 2I and Fig. 2J respectively. If the difference between $K_O^D$ (PlanetBuilder) and $K_O^D$ (Frost), is smaller than a specified uncertainty (default: $< 10^{-4}$), the hypothetical compositions of the planetary mantle and impactor core are considered to be in equilibrium (Fig. 2K). Otherwise, the solver will adjust the FeO mantle value (Fig. 2L). This process is repeated until the $K_O^D$ values of the Frost and PlanetBuilder models converge. The program then checks if (additional) corrections are necessary to account for the effects changes of the activity of elements in the molten impactor core have on $K_M^D$ (Fig. 2M). Any additional corrections are calculated with the $K_M^D$ values adjusted according to the procedure in Sect. 2.4 (Fig. 2N). If no (further) corrections are necessary, the solver returns the equilibrated major element compositions of the planetary mantle and impactor core as the final compositions. This enables the program to proceed with the calculations of the trace element distributions.

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### 2.4 Metal activity coefficients

An important aspect of our model is the option to correct the exchange coefficient $\mathrm{K}_{\mathrm{M}}^{\mathrm{D}}$ (Eq. 7) for changes in the activity of elements within the metal liquid of the impactor core. To calculate the corrections, we use the $\epsilon$ approach from Ma (2001), following the approach of Wade and Wood (2005) and Norris (2017).

The $\epsilon$ approach is an improvement on the old Wagner $\epsilon$ formalism (Wagner, 1952) by Ma (2001). It is used to describe the thermodynamic properties of a multicomponent system, an iron-rich metallic liquid in this case. The $\epsilon$ approach uses the interaction parameters ($\epsilon$) to describe the effect an element has on the activity coefficient ($\gamma$) of another element in the same liquid. The equations from Ma (2001) are split up into two parts: the calculation of the activity coefficient of the solvent (Eq. 23 from Ma (2001)) and the activity coefficients of the solutes (Eq. 24 from Ma (2001)). In our model the solvent is the Fe liquid of the impactor core and the solutes are the other elements present in liquid Fe. The equations from Ma (2001) then become:

$$
\begin{aligned}
\ln\gamma_{\mathrm{solvent}} = \ln\gamma_{\mathrm{Fe}} = & \sum_{i=2}^{N}\varepsilon_i^i(x_i+\ln(1-x_i)) \\
& -\sum_{j=2}^{N-1}\sum_{k=j+1}^{N} e_j^k x_j x_k\left(1+\frac{\ln(1-x_j)}{x_j}+\frac{\ln(1-x_k)}{x_k}\right) \\
& +\sum_{i=2}^{N}\sum_{\substack{k=2\\(k\neq i)}}^{N}\varepsilon_i^k x_i x_k\left(1+\frac{ln(1-x_k)}{x_k}-\frac{1}{1-x_i}\right) \\
& +\frac{1}{2}\sum_{j=2}^{N-1}\sum_{k=j+1}^{N}\varepsilon_j^k x_j^2 x_k^2\left(\frac{1}{1-x_j}+\frac{1}{1-x_k}-1\right) \\
& -\sum_{i=2}^{N}\sum_{\substack{k=2\\(k\neq i)}}^{N}\varepsilon_i^k x_i^2 x_k^2\left(\frac{1}{1-x_i}+\frac{1}{1-x_k}+\frac{x_i}{2(1-x_i)^2}-1\right)
\end{aligned}
\tag{47}
$$

$$
\begin{aligned}
\ln\gamma_{\mathrm{i}} = & \ln\gamma_{\mathrm{solvent}}+\ln\gamma_{\mathrm{i}}^0-\varepsilon_{\mathrm{i}}^{\mathrm{i}}\ln(1-\mathrm{x_i}) \\
& -\sum_{\substack{k=2\\k\neq i}}^{N}\varepsilon_i^k x_k\left(1+\frac{ln(1-x_k)}{x_k}-\frac{1}{1-x_i}\right) \\
& +\sum_{\substack{k=2\\k\neq i}}^{N}\varepsilon_i^k x_k^2 x_i\left(\frac{1}{1-x_i}+\frac{1}{1-x_k}+\frac{x_i}{2(1-x_i)^2}-1\right)
\end{aligned}
\tag{48}
$$

In both equations, $\gamma_{\mathrm{Fe}}$and $\gamma_{\mathrm{i}}$ are the activity coefficients of solvent Fe and solute *i* respectively. The interaction parameters $\epsilon_{\mathrm{i}}^{\mathrm{j}}$ refer to the effect element *i* has on the activity of element *j* in the Fe liquid. These values are dependent on the mole fractions of element *i* ($\mathrm{x_i}$) and *j* ($\mathrm{x_j}$). The $\gamma_{\mathrm{i}}^0$ value is a reference value for the activity coefficient if element *i* is in an infinite dilution in Fe liquid. Along with the $\epsilon_{\mathrm{i}}^{\mathrm{j}}$ values, the $\gamma_{\mathrm{i}}^0$ values are reference values that are typically determined at 1873K and extrapolated to higher temperatures using the approach from the Steelmaking Data Sourcebook (The Japan Society for the Promotion of Science, 1988):

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**Table 2.** Epsilon reference values for Ni, O and S

| $\epsilon_i^j$ | Ni | O | Si |
|---|---|---|---|
| Ni | 0.12[1] | 0[2] | 7.5[1] |
| O | 0[2] | −1[3] | −5[3] |
| Si | 7.5[1] | −5[3] | 8.6[1] |

1: Tuff et al. (2011); 2: Fischer et al. (2015); 3: Tsuno et al. (2013)

$$\ln \gamma_i^0(\mathrm{T}) = \frac{\mathrm{T}^0}{\mathrm{T} \cdot \ln \gamma_i \cdot \mathrm{T}^0} \tag{49}$$

$$\epsilon_i^j = \frac{\mathrm{T}^0}{\mathrm{T}} \cdot \epsilon_i^j \cdot \mathrm{T}^0 \tag{50}$$

where *T* is the temperature (in K) at which the metal-silicate equilibration occurs within the planetary mantle. The $\gamma_i^0$ reference values used in PlanetBuilder are based on values from (The Japan Society for the Promotion of Science, 1988; Norris, 2016; Tuff et al., 2011), as summarised in (Norris, 2017). Similarly, the $\epsilon_i^j$ reference values list originates from (Norris, 2017), although several important interaction values for Si, Ni and O have been updated based on more recent studies (Table 2). To ensure our model can be used for future work, both the $\gamma_i^0$ and $\epsilon_i^j$ reference values can be modified by the PlanetBuilder user.

As the metal activity coefficients are dependent on the metal liquid composition, they are susceptible to changes in the metal liquid compositions as well (Eq. 47 and 48). Continuously altering the activity coefficients at every iteration, while the planetary mantle and impactor core are not yet in equilibrium, creates a positive feedback loop where the solver derives a new composition for the impactor core based on the current activity coefficients, which are in turn modified by the new composition. To avoid this problem, the activity coefficients are only adjusted after potentially equilibrated compositions for the planetary mantle and impactor core are identified (Fig. 2N). This creates iteration cycles where the metal activity corrections are gradually adjusted. Each iteration cycle results in progressively smaller changes to the potentially equilibrated compositions and corresponding activity coefficients. Eventually this leads to an equilibrated planetary mantle and impactor core composition that fully accounts for the non-ideal mixing behaviour (Sect. 3.2). These equilibrated major element compositions are subsequently returned by the solver, allowing the model to continue with calculating the trace element concentrations.

### 2.5 Minor and trace element partitioning

The partitioning behaviour of minor and trace elements are calculated from Eq. (7), (10) and (11) using the major element concentrations. The $\mathrm{K_M^{App}}$ in Eq. (10) is calculated from the *PT* conditions of the accretion step. If ideal mixing behaviour is assumed, no corrections for activity behaviour have to incorporated and the $\mathrm{K_M^D}$ and $\mathrm{K_M^{App}}$ are considered equal. When taking non-ideal mixing behaviour into account, the $\mathrm{x_{Fe}^{metal}}$ from Eq. (43) is used to determine the $\gamma_{\mathrm{M}}^{\mathrm{metal}}$ following Sect. 2.4, and

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derive the $K_M^D$ from $K_M^{App}$ (Eq. 11). The $K_M^D$ is used with the equilibrated $x_{FeO}^{silicate}$ (Eq. 42) and $x_{Fe}^{metal}$ (Eq. 43) to calculate the partitioning behaviour of the minor and trace elements (Eq. 7).

### 2.6 Calculating the composition of the planetary core

The compositions of the equilibrated impactor core and planetary mantle can be used to calculate the new compositions of the planetary mantle and planetary core. To achieve this, the material of the remaining equilibrated impactor core is added to the planetary core. In case of partial equilibration, the non-equilibrating part of the impactor core is added to the planetary core prior to the equilibration process as well (Fig. 1.2C). The bulk mass, size and composition of the planetary core are altered without any further processes influencing it. The new compositions of the planetary mantle and planetary core are then stored by the model to be used as the starting compositions during the next accretion step.

## 3 Model validation and discussion

PlanetBuilder is designed to be versatile, capable of handling multiple different planetary and impactor compositions, metal-silicate equilibration conditions, partitioning data, and metal activity models. We validated its functionality by comparing the output of PlanetBuilder with the output of a canonical Earth accretion core model: the 'HET-2' model of Rubie et al. (2011). The 'HET-2' model of Rubie et al. (2011) describes a multi-stage core formation process for Earth, up to 98% of the current Earth's mass, divided into 24 discrete accretion steps. Rubie et al. (2011) used CI chondrite compositions from Palme and O'Neill (2003), enriched in several elements, to derive two sets of impactors: the first set is very reduced with relatively large metallic cores, the second set is more oxidised with smaller metallic cores and a mantle enriched in FeO. The transition between the two impactor sets occurs at accretion step 21 (after 67% of the Earth has accreted), and causes an abrupt change in the resulting planetary mantle and core compositions and size. A second, more subtle transition is introduced at accretion step 18 (55% Earth accretion), with a continuously decreasing degree of equilibration between the impactor core and planetary mantle. The canonical model of Rubie et al. (2011) assesses the behaviour of $Fe/FeO$, $Si/SiO_2$, $Ni/NiO$, O, Co, Cr, Nb, Ta, V and W. The compounds $Al_2O_3$, CaO and MgO are treated as present in the planetary and impactor mantle, but do not participate in the any partitioning processes. The 'HET-2' model also adds 2wt% S to the planetary core composition after partitioning is complete.

Implementing the 'HET-2' model conditions, compositions and parameters into our model, the PlanetBuilder output is in excellent agreement with Rubie et al. (2011), as shown in Supplementary Material S2. Minor differences are caused by two factors. First, we use a different normalisation as PlanetBuilder takes all major, minor and trace element abundances into account for its normalisation. Second, our program uses a more accurate MIDACO solver instead of an approximation to calculate the thermodynamic $K_O^D$. The dataset based on the 'HET-2' model from Rubie et al. (2011), with identical input parameters (*PTX*) and exchange coefficients ($K_M^D$) serves as a baseline to assess the effects of changing input parameters on the model outcome. Figure 3 specifically shows the effects of updating equilibrium constant parameterisations using experimental data produced after the publication of the Rubie et al. (2011) study (Table 1), including propagation of errors in such parameterisations; and

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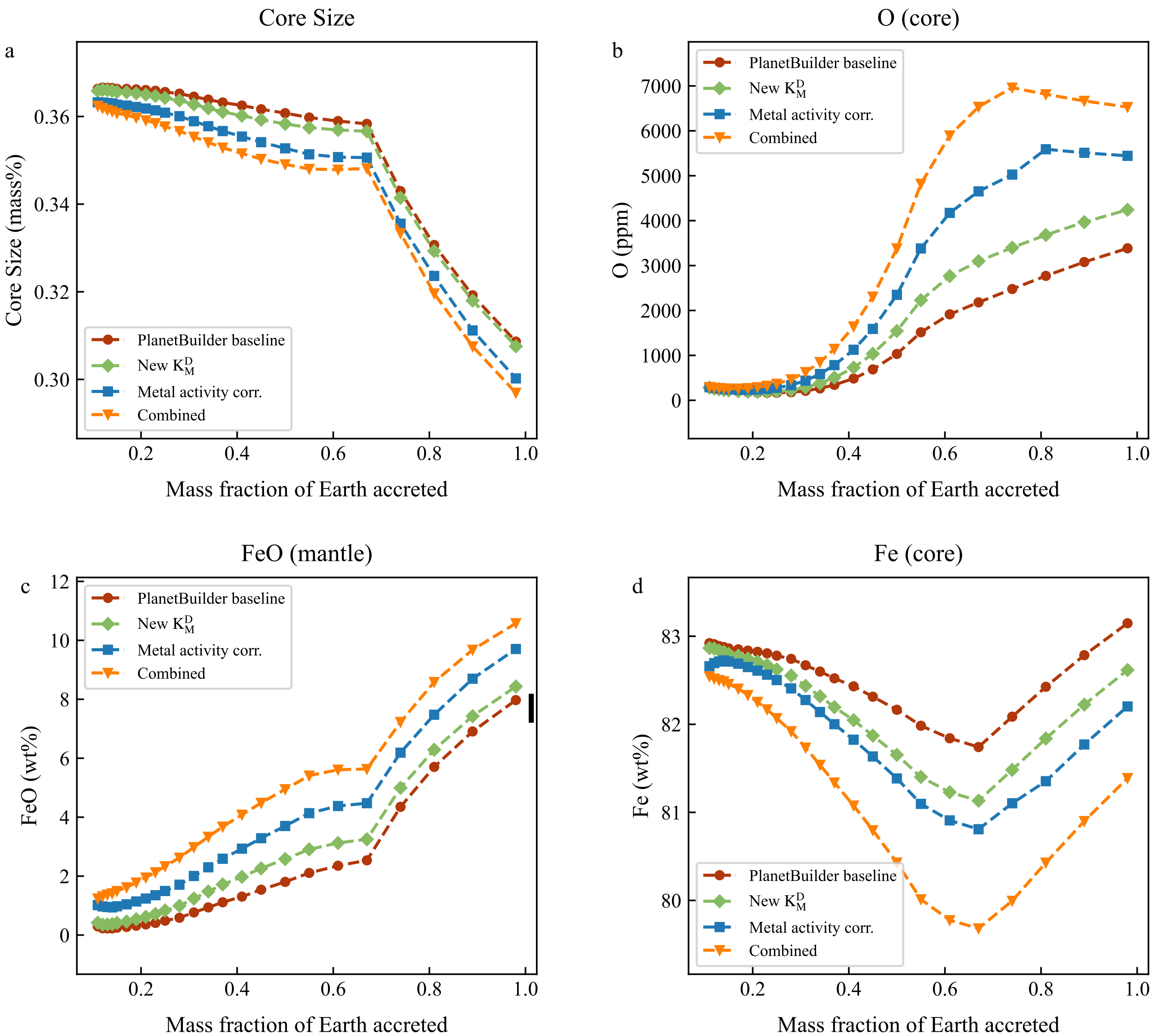
440 the effects of incorporating non-ideal behaviour of elements in liquid metal, which were ignored in the Rubie et al. (2011) study. The implications and significance of the data in this figure are discussed in Sect. 3.1 (equilibrium constants), Sect. 3.2 (metal activity corrections) and Sect. 3.3 (oxidised impactors).



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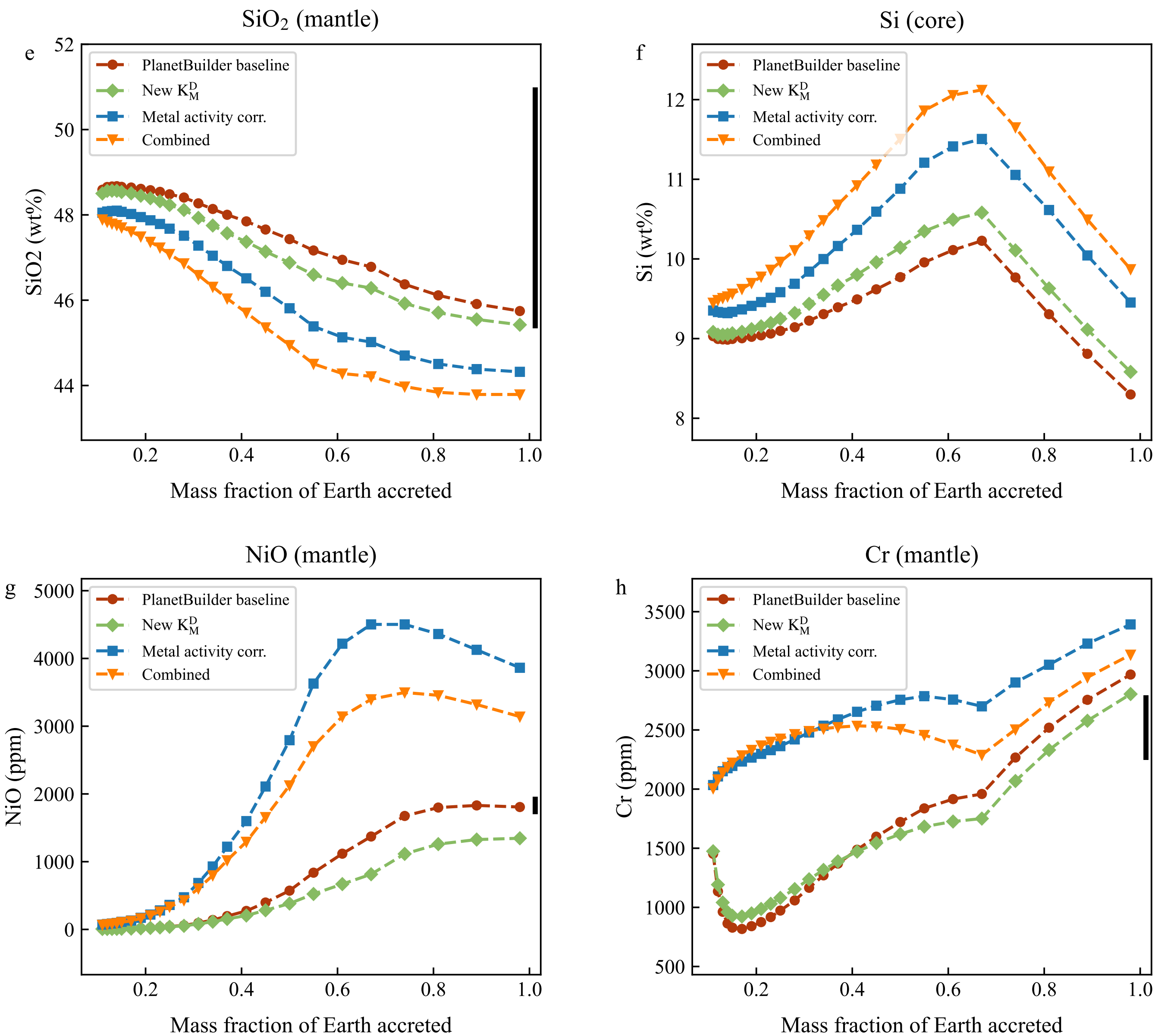


**Figure 3.** The influence of metal activity, new $K_M^D$ parameters and the combination of the two on the core size (a) and the concentrations of selected elements in the mantle and core (b-h). The black bars on the right-hand side of panels c, e, g and h show the range of bulk silicate Earth (BSE) abundance estimates for selected elements according to (Palme and O'Neill, 2014). Additional figures of the other elements taken into account, as well as the pressure, temperature, $fO_2$, $K_{Si}^D$ and $K_{Ni}^D$ can be found in Supplementary Material S1.

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### 3.1 The importance of equilibrium constants

Incorporating new experiemental data in the parameterisation of element partitioning through equilibrium constants $K_M^{App}$ (Table 1), have a significant impact on the equilibrated compositions of the Earth (Fig. 3). Whereas the canonical model of Rubie et al. (2011), shown as the baseline PlanetBuilder model in Fig. 3, mostly plots within the error margins of the measured composition of the bulk silicate Earth (BSE), the use of updated equilibration parameters causes most of modelled elemental abundances in the mantle to fall outside the uncertainty range of the composition of the BSE. This highlights the significant effect equilibrium coefficient parametrisations can have on the outcome of core formation models.

Propagation of errors in the metal-silicate partitioning parameterisations given in Table 1 can affect model results significantly (e.g. Walter and Cottrell, 2013). This effect can be seen in Fig. 4, which shows the evolution of the mantle and core concentrations of trace element Co in the growing Earth for the canonical baseline model. Varying the equilibrium constant parameterisation from Table 1 between ±1SD from the average leads to predictions of the Co concentrations in the BSE varying between 59-105 ppm and between 2440-2541 ppm for the planetary core. Whereas Co is a minor element, and variation in its equilibrium constants only significantly affect the partitioning of Co, variations in the equilibrium constants of a major element like Si affect the whole model. PlanetBuilder is very sensitive to changes in equilibrium constants and can therefore be used to evaluate new regression coefficients and their effects on the partitioning processes under various conditions($P$, $T$, $fO_2$) and compositions.

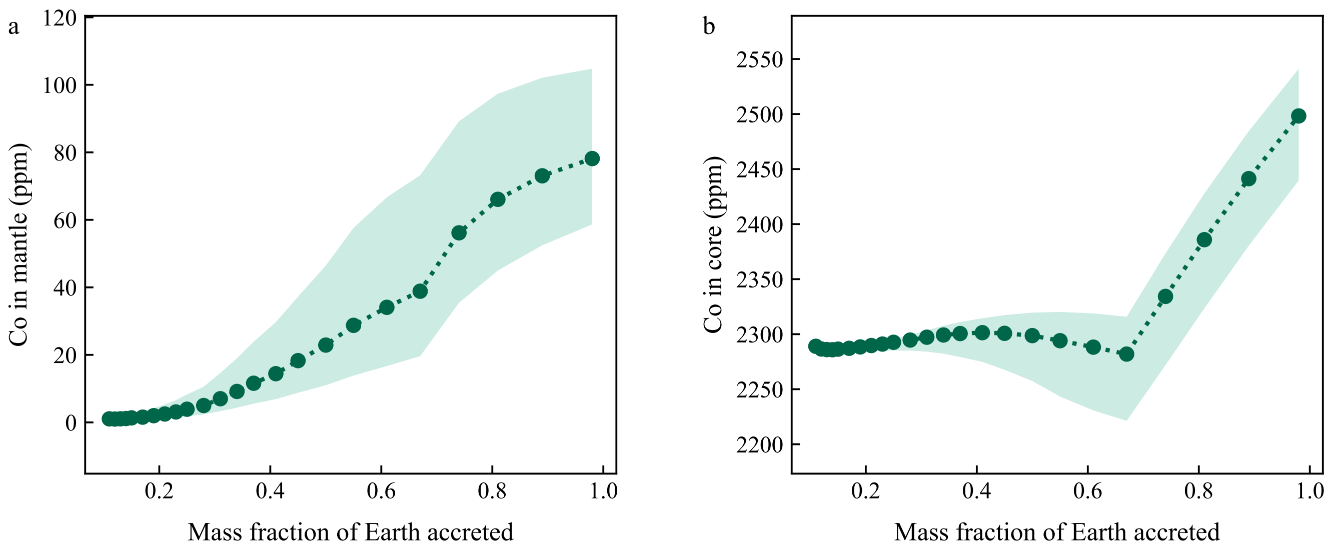


**Figure 4.** The concentrations of Co in the Earth's mantle and core for $K_{Co}^{D} \pm 1$ SD using the parameters from Fischer et al. (2015) from Table 1.

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### 3.2 Corrections for the activity of elements in metal liquid

The largest addition of PlanetBuilder compared to published multi-stage core formation models is the implementation of corrections for the equilibrium coefficients due to non-ideal activity behaviour within the metal (Fe) liquid. This results in a more complex partitioning behaviour, taking into account not only changes in *PT* conditions for determining the equilibrium constants, but also compositional changes. As mentioned in Sect. 2.4, the solver calculates the metal activity corrections in cycles to gradually find an equilibrated composition with corresponding $\mathrm{K_M^D}$ values that are corrected for non-ideal mixing behaviour. However, the increments with which the activity corrections are adjusted are not arbitrary (Fig. 5). Large increments tend to require fewer iteration cycles to reach the equilibrated compositions with appropriately corrected $\mathrm{K_M^D}$ values, but this only works for relatively simple compositions. To account for this, the solver will automatically adjust the increment size if no solutions are found within the specified 1-hour timeframe. When the equilibrated composition and $\mathrm{K_M^D}$ values remain constant over multiple cycles (default: fluctuation of $< 10^{-3}$ over 10 cycles for all elements and $\mathrm{K_M^D}$ values), the solver will return the results.

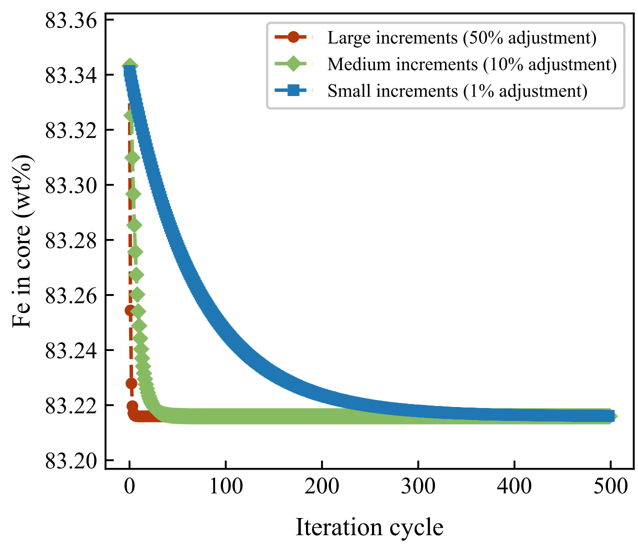


**Figure 5.** Example of the stabilisation of the composition (approximated by the evolution of calculated FeO abundance in the mantle) and $\mathrm{K_M^D}$ with incremental changes to the metal activity corrections. Increments are expressed in percentage adjustment of the $\mathrm{K_M^D}$ values based on the suggested corrections: a 10% increment means that after each iteration cycle, new corrected $\mathrm{K_M^D}$ values are calculated, and the current $\mathrm{K_M^D}$ values are shifted 10% in that direction for the next iteration cycle.

Figure 3 shows that the addition of the metal activity corrections for non-ideal mixing behaviour have a significant impact on the partitioning of all major and minor elements. Whereas the canonical model of Rubie et al. (2011), which did not incorporate metal non-ideality, yields mantle element abundances largely in agreement with BSE compositions, this is no longer the case once non-ideality in metal liquid is assumed. For example, the final Cr mantle abundance in the Earth in the canonical baseline

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model using input parameters from Rubie et al. (2011) changes from 2804 ppm to 3392 ppm when including corrections for non-ideal behaviour, a change of approximately $+17.3\%$. Mantle element abundances for the elements considered by Rubie et al. (2011) overall vary with -4.5% to +48%, and the final values for most elements (FeO, $SiO_2$, NiO, Cr, Co, V and W) fall significantly outside the observed BSE abundance range once non-ideality corrections are incorporated. This implies that models previously considered successful in the absence of activity corrections could become unsuccessful when metal activity effects are considered.

It is worth to note that the interaction- and activity coefficients ($\epsilon$ and $\gamma$ respectively) are two types of parameters that still require improvement. As discussed in Sect. 2.4, the reference values for $\epsilon_{\mathrm{i}}^{\mathrm{j}}$ and $\gamma_{\mathrm{i}}^{0}$ are derived at 1873K from the steelmaking industry, and are extrapolated to higher temperatures. This approach often assumes a linear relationship between the parameters and inverse temperature, using Eq. 50 and Eq. 49, based on thermodynamics (The Japan Society for the Promotion of Science, 1988). Although this is a good approximation, there is no direct evidence for this relationship at temperatures appropriate for core formation within large planetary bodies. Core formation also occurs at significantly higher pressure than encountered in the steelmaking industry, and the current extrapolation assumes that $\epsilon_{\mathrm{i}}^{\mathrm{j}}$ and $\gamma_{\mathrm{i}}^{0}$ are completely unaffected by changes in pressure. When extrapolating the reference values to temperatures of over 3000K for core formation, even the smallest deviations from the linear relationship can result in inaccurate values. Combined with the extrapolation of the error margins of the reference values for $\epsilon_{\mathrm{i}}^{\mathrm{j}}$ and $\gamma_{\mathrm{i}}^{0}$, this introduces a significant uncertainty in the extrapolated values and ultimately in the outcomes of our model as well. New insights in these reference values, their behaviour and their extrapolation to higher temperatures and pressures will therefore help to improve the accuracy of PlanetBuilder.

### 3.3 Oxidised impactors

Several studies indicate that in the late stages of the accretion process for Earth and several other rocky planets, impactors may have become more oxidised (e.g. Wanke and Dreibus, 1988; O'Neill, 1991; Siebert et al., 2013; Righter et al., 2017). These oxidised impactors are characterised by higher FeO contents in their silicate mantles and relatively smaller metallic cores compared to less oxidised impactors. During the accretion processes, these impactors introduce significantly larger amount of oxygen into the modelled planetary system. This poses a unique challenge for core formation models, including PlanetBuilder, as our equilibration process balances the partitioning of oxygen between impactor core and planetary mantle. When the impactor mantle is very enriched in FeO, a large portion of Fe partitions into the impactor core during equilibration. Substantial oxygen has to partition into the metallic liquid alongside the Fe to match experimentally observed oxygen partitioning behaviour. Since the impactor cores of oxidised impactors are relatively small, especially when partial equilibration is also taken into account, this can lead to an unrealistically oxidised metal liquid (e.g. Rubie et al., 2004). This problem was identified by Rubie et al. (2015), who stated that, in this situation, the impactor core should be treated as an oxide liquid rather than of a metal liquid. Without any metal liquid, the metal-silicate partitioning processes of core formation stops, and the oxide liquid is added to the planetary mantle. To accommodate for this, our model continuously tracks the amount and concentration of oxygen present in the metallic impactor core. If there is enough oxygen to oxidise all the Fe present, as per Eq. 3, the impactor core is considered too oxidised and is instead added to the planetary mantle.

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When assuming ideal activity behaviour of elements in the metal liquid, there are no problems with extreme oxidation in the 'HET-2' dataset (Fig. 3.b). However, this is not the case when the non-ideal metal activity behaviour is considered. During the accretion of the final series of oxidised impactors, the modelled metal liquid quickly turns into an oxide liquid (Sect. 3). The effects of the addition of this oxide liquid to the planetary mantle can also be observed in Fig. 3. Without additional supply of oxygen originating from the equilibration processes, the oxygen concentration of the Earth's core stabilises at approximately 9.6wt%.

## 4 Assumptions and limitations of the model

Aside from the challenges posed by oxidised impactors, there are several other assumptions and limitations in PlanetBuilder that should be considered. Although some of these limitations can be overcome by e.g. developing additional modules or further expanding the current model, this is not the case for several assumptions inherent to core formation modelling and PlanetBuilder itself.

Our model assumes the presence of one or more deep magma oceans in the planetary mantle to allow efficient equilibration reactions between the silicate liquid of the planetary mantle and Fe-liquid of the impactor core. As we only calculate the bulk compositions of the planetary mantle and planetary core, the model makes no assumptions regarding the timeframe, continuity, and size of the magma ocean(s). It is only required that a magma ocean, during the time of the equilibration processes, reaches the depth where the equilibration takes place. To ensure there is no re-equilibration between the planetary mantle and planetary core, the magma ocean should be accompanied by an underlying layer of solid mantle. The planetary core is considered a semi-closed reservoir: material from impactors can be added to it after the partitioning processes, but the planetary core never interacts with the solid mantle during accretion.

Similar to the planetary core, the planetary body itself is considered a semi-closed system as well. Impactors can be added to the planetary body, but the current model does not incorporate any methods for removing material from the planetary body, for example through outgassing and atmospheric escape processes. Although volatile elements and their partitioning behaviour can readily be added to the model, the absence of outgassing processes is a weakness. The potential addition of outgassing processes comes with its own assumptions and limitations. Volatiles are expected to dissolve in silicate melts under high pressure deep within the mantle, but exsolve near the planetary surface or during large impacts where there is a local increase in heat. Therefore, most of the devolatilisation is expected to occur near the planetary surface during large impacts. The conditions and events on any depth other than the one associated with the effective pressure of the equilibration processes, are not part of our model. It is possible to combine our model with other models that e.g. include devolatilisation of impactors. Calculating the loss of volatiles within impactors before or during the accretion processes, prior to it sinking through the magma ocean, only alters the amount of material that is added to the planetary body. This does not affect the functionality of the equilibration processes deep within the magma ocean. However, devolatilisation of the planetary body during impacts is more complicated due to the presence of oxygen. Oxygen is the only volatile element present in our model and its partitioning between planetary mantle and impactor core is the most important variable of the solver (Sect. 2.3.1). The model assumes all oxygen added to

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the planetary body remains there. As explained in Sect. 3.3, making any assumptions regarding the partitioning of oxygen will significantly affect the equilibration processes. The same result is expected if any assumptions are made regarding the outgassing of the oxygen already present in the planetary body.

The planetary bodies and impactors in our model are anhydrous. Whilst the addition of hydrogen and its partitioning would ideally be combined with the addition of outgassing processes, the presence of hydrogen in the planetary system is known to affect the metal-silicate partitioning processes as well (Clesi et al., 2016; Tagawa et al., 2021; Huang et al., 2026). Hydrogen modifies the partitioning behaviour of major elements such as $\mathrm{Fe}$ and $\mathrm{Ni}$, and accommodating for hydrous conditions would therefore require significant adjustments to the solver in the model.

The current version of our model cannot be used to model chalcophile behaviour or sulfide-liquid partitioning processes. The presence of sulfur strongly alters the geochemical behaviour of various major and minor elements, as the silicate-sulfide and metal-sulfide partitioning behaviour significantly affect the metal-silicate partitioning behaviour. Sulfur-rich systems cause lithophile elements to segregate into a sulfide-liquid, and these silicate-sulfide transitions vary with pressure, temperature and oxygen fugacity (e.g. Boujibar et al., 2014; Wood and Kiseeva, 2015; Wood et al., 2014; Steenstra et al., 2020). Incorporating such behaviour with extensive consequences for the metal-silicate partitioning of all elements into a geochemical model requires further systematic assessment of all variables involved.

## 5 Model possibilities

The main advantages of our model are its accessibility, modularity, and possibility to incorporate metal activity corrections. As an open-source model, other scientists who might not have chemical modelling tools available, can freely use our model to test their data and new ideas. This provides experimental studies, for example, with the possibility to model the implications of their experimental results without having to invest time in the creation of an extensive chemical multi-stage core formation model.

The focus on calculating the bulk compositions of the mantle and core of the planetary body, means that our model can serve as a starting point or addition to other models, both geochemical and geophysical. Our model can improve current bulk composition estimates that are used as the input for e.g. mantle dynamics, magma ocean solidification and crystallisation models. Since it is not necessary to simulate the full planetary growth in a single run, it is possible to model the influence of a small set of impactors on a still growing planet or export the data after a certain fraction of the planetary body has formed.

Our model has many possibilities to grow by incorporating new ideas and insights. It is extremely sensitive to small changes in the $\mathrm{K_M^D}$ and $\mathrm{K_M^{App}}$ (Sect. 3.1), especially when including corrections for non-ideal activity of elements in a Fe-liquid (Sect. 3.2). This sensitivity makes our model very useful for reviewing the influence that potential new equilibration constants, partitioning-, interaction- and activity coefficients might have on model outcomes.

Although the current model includes a total combination of 10 major, minor and commonly used trace elements, additional elements can be added if their partitioning behaviour is known. With the exception of the elements mentioned in Sect. 4, adding new lithophile elements or elements that partition after the equilibration of $\mathrm{Fe}$, $\mathrm{Si}$, $\mathrm{Ni}$ and $\mathrm{O}$ is relatively straight-forward. The

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included list of interaction- and activity coefficients is more extensive than the currently included elements, but might require updating to account for new published data.

The modular programming approach supports not only the addition of new elements and parameters for equilibrium constants, but also the addition of new modules. It is important to keep in mind that the model can be used over a large range of pressures, temperatures, and compositional changes that are associated with rocky planetary growth. Therefore, any addition should either provide accurate data for the same range or be used only for a limited data-set.

In this paper we consistently refer to the resulting data as the planetary mantle and planetary core to avoid confusion. However, the resulting body need not necessarily be a planetary body. It is possible to model the evolution of any rocky body that grows through accretion processes. This might include the core formation of e.g. differentiated meteorites, planetary satellites or simply theoretical compositions. Therefore, our model can be used for studying exoplanets and their potential compositions, on top of the rocky planetary bodies present in our solar system.

## 6 Conclusions

In summary, PlanetBuilder is an open-source geochemical multi-stage core formation model specialised in calculating the chemical bulk compositions of rocky bodies like the Earth with a complex accretion history, through mass balance and metal-silicate partitioning. Our model is designed to be modular and adjustable to provide scientists without chemical modelling tools available, the option to test their data and ideas. PlanetBuilder is very sensitive to changes in parameters such as equilibrium constants and activity coefficients, making it a useful tool for studying the effects any changes in these parameters might have on the partitioning behaviour and resulting compositions.

We have included the option to correct the partitioning coefficients for non-ideal behaviour of elements in iron liquid, which significantly alters the partitioning behaviour and the resulting composition. Our comparison of ideal and non-ideal activity behaviour on the same dataset indicates that core formation models that were considered successful without corrections for non-ideality might be unsuccessful when including these corrections and require revision.

*Code availability.* The PlanetBuilder 1.0 version is available on https://doi.org/10.5281/zenodo.19402406 (Seegers et al., 2026), under the GNU General Public License v3.0 licence. The MIDACO library used for the solvers is not included and can be found on the official MIDACO website: https://www.midaco-solver.com/

*Author contributions.* AS: methodology, software and writing - orignal draft. PV and WW: conceptualisation, funding acquisition, supervision and writing - review and editing.

*Competing interests.* The authors declare that they have no conflict of interest.

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