Dust Condensation in Evolving Discs and the Composition of Meteorites, Planetesimals, and Planets

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ABSTRACT

Partial condensation of dust from the Solar nebula is thought to be responsible for the diverse chemical compositions of the rocky planets/planetesimals in the inner Solar system. Here we present a forward physical-chemical model of a protoplanetary disc to predict the chemical compositions of planetesimals that may form from such a disc. Our model includes the physical evolution of the disc and the condensation and partial advection and decoupling of the dust within it. The condensation of the dust is calculated by a Gibbs free energy minimization technique assuming chemical equilibrium. We show that the chemical composition of the condensate changes with time and radius. A simple model based on the 50% condensation temperatures \( T_{50} \) predicts compositions of resulting planetesimals that are broadly consistent with those of CM, CO, and CV chondrites provided that the decoupling timescale of the dust is on the order of the evolution timescale of the disc or longer. If the decoupling timescale is an order of magnitude shorter than the evolution timescale of the disc then the calculated chemical compositions of planetesimals significantly deviate from the measured values. The relative elemental abundances in the condensed dust are highly affected by the thermal history of the disc. Our model can explain the chemical compositions of some of the terrestrial planets in the solar system and may constrain the potential chemical compositions of rocky exoplanets.

Key words: stars: pre-main-sequence – accretion, accretion discs – astrochemistry – solid state: refractory – solid state: volatile

1 INTRODUCTION

Our Solar system is an important testbed for studying the process of planet formation. Chemical compositions of terrestrial planets and both differentiated and undifferentiated meteorites can help constrain its formation and evolution. All terrestrial planets and many carbonaceous chondrites (CM, CO, and CV) are depleted in volatile elements and enriched in refractory elements relative to the composition of the Sun (as represented by CI chondrites (Asplund, Grevesse & Sauval 2005)). The degree of depletion of these elements is correlated with their volatility (Palme, Lodders & Jones 2014).

Figure 1 shows the relative elemental abundances of terrestrial planets and a number of carbonaceous chondrites normalized to the CI chondrites,

\[
R_j = \frac{[\chi_E / \chi_{Si}]_P}{[\chi_E / \chi_{Si}]_{CI}}
\]

as a function of the “50% condensation temperatures” \( T_{50} \), the temperature where half of a given element is in the condensed phase under a total pressure of \( 10^{-4} \) bar with a Solar composition for each element as tabulated in Lodders (2003). Here, \( \chi_E \) and \( \chi_{Si} \) stand for the concentrations of an element and Si, respectively, and subscript P refers to a planet or meteorite. \( R_j \) for terrestrial planets and CM, CO, and CV chondrites are smaller than unity for volatile elements while larger than unity for refractory elements. Determining causes of volatile element depletion in rocky planets, as well as the role that the physical and chemical environment plays in producing this depletion, is crucial for our understanding of the origin of our Solar system and is the subject of ongoing research in planetary science.

The volatile depletion in rocky planets (Figure 1) is commonly attributed to a partial condensation of dust in...
1.1 Previous work

Grossman (1972) was among the first to use a thermodynamic approach to study the chemical evolution of the solar nebula and the condensation of dust. He suggested that the CAIs are direct condensates from the nebula. Lewis (1974) applied the same concept to understand the chemical composition of the terrestrial planets.

Cassen (1996) modeled the chemical evolution of an evolving disc to explain the depletion of the volatile elements in CM, CO, and CV chondrites. He assumed that an element begins to condense once the temperature at a given radius in the disc drops below $T_{\text{eq}}$ at a pressure of $10^{-4}$ bar. Despite this simplifying assumption, he was able to broadly reproduce the volatile element depletions in carbonaceous chondrites by forming them between 1-3 AU.

Using the commercial software package HSC Chemistry, Bond, Lauretta, & O'Brien (2010a) calculated the equilibrium partitioning of 16 elements among 78 gaseous and 33 solid species at seven specific times in the evolving disc. They then modeled the formation of the terrestrial planets using N-body accretion simulations (O'Brien, Morbidelli & Levison 2006). Using the same method and different initial chemical compositions of host stars, Bond, O'Brien, & Lauretta (2010b) also modeled the formation of extrasolar planets. They showed that the resulting compositions of exoplanets are diverse, changing from Earth-like to carbide-rich planets.

Using the HSC Chemistry software package, three different disc models, and elemental abundances of the present-day solar photosphere (Asplund, Grevesse & Sauval 2005), they showed that the resulting compositions of exoplanets are diverse, changing from Earth-like to carbide-rich planets.

Figure 1. Observed elemental abundances: Relative abundances, $R_i$, in terrestrial planets and CM, CO, and CV chondrites, normalized to the CI chondrites and Si, as a function of $T_{\text{eq}}$ (Lodders 2003). Data sources: chondrites (Wasson & Kallemeyn 1988), bulk silicate Mercury (Morgan & Anders 1980), bulk silicate Venus (Morgan & Anders 1980), bulk silicate Earth (McDonough & Sun 1995), and bulk silicate Mars (Lodders & Fegley 1997). The horizontal line at 1 indicates where a body is neither enriched nor depleted in a given element. Horizontal dashed lines show the median depletions in these objects at $T_{\text{eq}}$ above and below 1310K. This figure shows that all terrestrial planets and chondrites are depleted in volatiles, and are consequently enriched in refractory elements relative to the Sun. Highly siderophile elements in Earth are not plotted because they were affected by core formation. Elements in red font are modeled by us using the GRAINS code (See Section 4 for introduction of the GRAINS code).
Elser, Meyer, & Moore (2012) modeled the development of the terrestrial planets composition. They adopted a self-consistent approach to determine the time in the evolving disc for calculations of radial variations in disc chemistry assuming chemical equilibrium. They showed that the chemical gradients in the system are affected by the disc models and the initial planetesimal disc masses.

Moriarty, Madhusudhan, & Fischer (2014) took into account both the evolution of disc and chemical equilibrium in it to investigate the compositions of the rocky planets around stars with different chemical compositions. They found a good agreement with previous studies for Sun-like stars with C/O \sim 0.54 and predicted a number of carbon-rich planets around stars with C/O > 0.65.

Pignatale et al. (2016) adopted a two dimensional disc model and used the HSC Chemistry software package which included 170 gases and 317 solids that form from 15 elements. A snapshot of the disc at 1 Myr was used as a proxy for typical disc conditions (temperature and pressure in the midplane of the disc) for modeling chemical and mineralogical gradients in the disc.

Given this background, none of these previous simulations take into account the simultaneous physical and chemical disc evolution, and they do not consider the effects of differential transport of gas and dust during the disc evolution. As the disc evolves with time, the surface density, temperature, and pressure in the disc change, which affects the condensation temperatures of chemical elements. Therefore, a time-dependent disc model is needed that considers the effects of changing pressure and surface density on the condensation temperatures over time for each radial distance of the evolving disc.

In this work, we use a modified evolving disc model from Cassen (1996) and the GRAINS code from Petaev (2009) to model chemical compositions of the gaseous and condensed phases at each time step and each radius. The GRAINS code calculates equilibrium partitioning of 33 elements (Table 1) among 242 gaseous and 520 solid compounds. As the disc evolves, the elements that condense from a parcel of disc gas at given T-P-r conditions will, over time, decouple from the gas and be retained at a given radius. Meanwhile, those elements left in the gas phase, and a portion of the dust that does not decouple (the “advecting dust”), continue to move with the gas. In these simulations we calculate the evolution and the final relative abundances of the elements in the decoupled dust—the building blocks of planetesimals.

2 ALGORITHM OVERVIEW

In our calculations, the elements will be in one of three different states: a gaseous phase, and one of two condensed phases—advecting dust and decoupled dust. The elements condense from the gas based upon the temperature of the disc midplane—either via the chemical equilibrium calculation, or by assuming it condenses at their respective T_{50}. The dust phase then decouples from the gas on a timescale proportional to the local orbital period (see Equations (9), (10), and (11)). As the disc evolves, the elements of the gas in gaseous phases follow the gas. Similarly, the portion of the dust that has not decoupled from the gas, the advecting dust, also follows the evolution of the gas.

Table 1. The 50% condensation temperatures from different models

| element | GRAINS(a) | GRAINS CT(b) | Lodders(c) | Cassen(d) |
|---------|-----------|--------------|------------|-----------|
| H       | ...       | ...          | ...        | ...       |
| He      | ...       | ...          | ...        | ...       |
| C       | ...       | 40           | ...        | ...       |
| N       | ...       | 123          | ...        | ...       |
| O       | ...       | 180          | ...        | ...       |
| Na      | 988       | 1069         | 958        | 971       |
| Mg      | 1336      | 1385         | 1336       | ...       |
| Al      | 1654      | 1675         | 1653       | ...       |
| Si      | 1316      | 1478         | 1310       | 1311      |
| P       | 1318      | 1358         | 1229       | 1151      |
| S       | 669       | 711          | 664        | 652       |
| Cl      | 440       | 446          | 948        | ...       |
| K       | 906       | 1014         | 1006       | 1002      |
| Ca      | 1500      | 1669         | 1517       | ...       |
| Ti      | 1583      | 1594         | 1582       | ...       |
| Cr      | 1304      | 1358         | 1296       | 1276      |
| Mn      | 1154      | 1263         | 1158       | 1191      |
| Fe      | 1335      | 1360         | 1334       | ...       |
| Co      | 1350      | 1361         | 1352       | ...       |
| Ni      | 1264      | 1326         | 1353       | 1354      |
| Cu      | 1100      | 1232         | 1037       | 1038      |
| Ga      | 1018      | 1159         | 968        | 920       |
| Ge      | 911       | 1062         | 883        | 826       |
| Mo      | 1548      | 1644         | 1590       | ...       |
| Ru      | 1544      | 1630         | 1551       | ...       |
| Pd      | 1336      | 1360         | 1324       | 1334      |
| Hf      | 1730      | 1749         | 1684       | ...       |
| W       | 1788      | 1832         | 1789       | ...       |
| Re      | 1770      | 1830         | 1821       | ...       |
| Os      | 1809      | 1833         | 1812       | ...       |
| Ir      | 1584      | 1691         | 1603       | ...       |
| Pt      | 1396      | 1509         | 1408       | ...       |
| Au      | 1196      | 1322         | 1060       | 1224      |

(a) T_{50} calculated from the GRAINS Code. If T_{50} for an element is less than 300 K, we do not provide it here. (b) The condensation temperatures calculated from the GRAINS Code. When the amount of an element in the condensed phase is larger than 2% of the total amount of the element, we define the corresponding temperature as the condensation temperature. (c) T_{50} showed in Lodders (2003). (d) T_{50}s used in Cassen (1996). Here the pressure is 10^{-4} bar.

The portion of the dust that decouples no longer interacts chemically with the surrounding elements, and it no longer interacts with the gas disc—remaining at the location where it condensed. As the advecting dust is transported into new regions, we assume it is brought into chemical equilibrium with the ambient material and we use the new composition to calculate the new abundances of the condensed material. Figure 2 is a flowchart that shows how our algorithm tracks the chemical composition of the decoupled dust in the disc midplane.

3 GASEOUS DISC EVOLUTION MODEL

For this work, we adopt the disc model used by Cassen (1996) to calculate the evolution of the gaseous disc (H$_2$ and He). In this model, the surface density at semi-major
axis $r$ and time $t$ is given by

$$\Sigma(r, t) = \Sigma_0(t) \exp(-[r/r_0(t)]^2).$$

Here $\Sigma_0(t)$ is the surface density near the central star, which is

$$\Sigma_0(t) = \frac{M_d}{\pi r_0^2},$$

and $r_0(t)$ is the characteristic radius, which is given by

$$r_0(t) = \frac{1}{GM_\odot} \left( \frac{J}{M_d \Gamma_{5/4}} \right)^2,$$

where $M_d$ is the mass of the disc, $G$ is the gravitational constant, $M_\odot$ is the mass of the central star (in this paper, we use $1 M_\odot$), $J$ is the angular momentum of the disc (we adopt $J = 3 \times 10^{52}$ g cm$^2$ s$^{-1}$), and $\Gamma_{5/4}$ is 0.9064.

The evolution of the disc mass is governed by

$$M_d(t) = M_{d0} \left( 1 + \frac{t}{t_c} \right)^{-0.5},$$

where $M_{d0}$ is the mass of the disc at $t = 0$ and $t_c = 2.625 \times 10^4$ yr is the characteristic evolution timescale of the disc.

The midplane of the disc is heated by the accretion of the gas, so the midplane temperature, $T(r, t)$, can be calculated from (Cassen 1994)

$$T = \frac{3GM_\odot \dot{M}}{6\pi \kappa SB r^3},$$

where $\dot{M}$ is the mass accretion rate to the central star, $\sigma SB$ is the Stefan-Boltzmann constant, and $\kappa = \kappa SB$ is the optical depth ($\kappa = 4 \text{ cm}^2 \text{ g}^{-1}$ is the opacity of gas with solar abundance).

The midplane pressure is

$$P = \frac{\rho RT}{\mu},$$

where $\rho$ is the density, $R$ is the gas constant, $\mu = 2.34$ is the mean molecular weight, $\rho = \Sigma/\sqrt{2\pi} H$ is the midplane density, and $H$ is the scale height of the gaseous disc.

For all the remaining elements in gas phase, we assume that they have the same velocity as the H$_2$ and He. Their evolution is governed by

$$\frac{\partial \Sigma_i}{\partial t} + \frac{1}{r} \frac{\partial (r V_r \Sigma_i)}{\partial r} = 0,$$

where $\Sigma_i$ is the surface density of elements $i$ in gas phase and $V_r$ is the radial velocity of H$_2$ and He.

Figure 3 shows how the gaseous disc evolves with time. Figure 3 (a) shows the evolution of the normalized surface density of the disc. As time goes on, the surface density decreases in the inner region (radii less than several AU) while it increases in the outer region of the disc (i.e., the disc expands). The general trends of temperature (see Fig. 3 (b)) and pressure (see Fig. 3 (c)) with time are similar to the trend of surface density. Note that the temperatures at radii interior to 4 AU always decrease with time.

4 RECALCULATING 50% CONDENSATION TEMPERATURES WITH GRAINS

We calculate the chemical equilibrium during the disc evolution with the GRAINS code (Petaev 2009) under local chemical and physical conditions. The elements used in the GRAINS code are shown in Table 1. In this case, H and He account for 98.65% (H: 71.34%, He: 27.31%) of the total mass with the remaining elements having Solar abundances (Lodders 2003). GRAINS distributes 33 elements among 242 gaseous and 520 solid species by minimizing the Gibbs free energy of the system to identify the chemical equilibrium composition.

Cassen (1996) and Lodders (2003) estimate their $T_{50}$ based upon a single pressure of $10^{-3}$ bar. However, the $T_{50}$ depends upon the starting composition and the pressure (which, in turn, affects the condensation process throughout the disc). Here, we recalculate $T_{50}$ for each element by fixing the value of pressure (from $10^{-12}$ to 1 bar) and lowering the temperature from 2500 K to 300 K to follow the
condensation sequence. We note that this calculation does not involve the disc evolution—so there are only the gas and dust phases. $T_{50}$ for each element is the temperature when the amount of the element in the gas phase equals that in the dust phase. Figure 5 shows the effect on the $T_{50}$ of the elements when changing the pressure from $10^{-12}$ to 1 bar. The proportions of several elements that are in the gaseous and dust phases as functions of temperature are shown in Figure 5. The temperature intervals over which the various elements condense are different for each elements.

In Figure 5 (a), we see that $T_{50}$ for Mg, Si, and Fe are 1336, 1316, and 1335 K, respectively. Due to the different condensation temperature intervals (the difference between the temperatures at which an element begins to condense and condenses completely), the element with lower $T_{50}$ may have higher relative abundance in the dust phase at certain temperatures. For example, at temperatures between 1350 and 1500 K, the relative abundance of Si in the dust phase is more than those of Mg and Fe as shown in Figure 5 (a). When the pressure of the system increases, the $T_{50}$ also increase. However, the relative values of $T_{50}$ may also change. For example, consider Si and P, $T_{50}$ for Si is higher than that for P when the pressure $P = 1 \times 10^{-12}$ bar while the value for Si is relatively low when $P = 1$ bar.

We compare $T_{50}$ calculated from the GRAINS code with those used in Cassen (1996) and in Lodders (2003) in Figure 6. The values are generally consistent with each other, though several individual elements have quite differ-

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Figure 3. Disc evolution: (a) Normalized surface density ($\Sigma_0$ is the initial value of $\Sigma_0$), (b) Midplane temperature, and (c) Midplane pressure for the disc at various points in time. (d) Radial velocity of the gas.

Figure 4. 50% condensation temperatures: $T_{50}$ as a function of elements for various pressures (a) and pressure for various elements (b).
The relative abundances of each element match the solar composition and the gas phase as a function of the midplane temperature. The relative Mg, Al, Si, P, K, Ca, Ti, and Fe) in the condensed phases and the gas phase.

Figure 6. Updated 50% condensation temperatures:

Our first model comparison is between the original work of Cassen (1996) and a similar model where we use new values for $T_{50}$ that we calculated using the GRAINS code (and which we just described). In both models that use $T_{50}$, a given element does not start to condense until temperature drops below its corresponding $T_{50}$.

These models are only an approximation as in every case, an element condenses over a range of temperatures. We improve upon this assumption in the second new model (M2), where we calculate the chemical equilibrium of the 33 elements at each point in time in the evolving disc at each radius. In each of these three models, the solids decouple out of the disc in each timestep while the remaining gaseous and advecting dust portions are transported the along with the disc materials. We give details of the two new models in the following sections.

5.1 Model 1: Updated 50% condensation temperatures from the GRAINS code

Our first model comparison is between the original work of Cassen (1996) and a similar model where we use new $T_{50}$ derived from the GRAINS code. (See Table 5 and Figure 6 for $T_{50}$ of both models.) In this model, when the temperature at a point in the midplane of an evolving disc is less than $T_{50}$ for an element, the element will begin to condense and decouple. The amount of the decoupled dust is determined by the decoupling rate,

$$
\frac{d\sigma_i}{dt} = \begin{cases} 
0, & \text{when } T > T_i, \\
\epsilon \Omega \Sigma_i, & \text{otherwise,}
\end{cases}
$$

(9)

where $\sigma_i$ is the surface density of element $i$ in the decoupled dust, $T_i$ is the $T_{50}$ for element $i$, $\epsilon$ is the decoupling efficiency, $\Omega$ is the angular velocity around the central star, and $\Sigma_i$ is surface density of element $i$ in the advecting dust. If $T < T_i$, then $\Sigma_i$ equals the surface density of element $i$ in the gas phase.

The decoupling efficiency is uniform across the entire disc. The decoupling timescale at 1 AU is given by

$$
\tau_{\text{dec}} = \frac{1}{\epsilon \Omega (r = 1\text{AU})}.
$$

(10)

We normalize the decoupling time at 1AU and the time for the dust to decouple at different distances depends upon the local orbital speed. A decoupling timescale of zero corresponds to immediate decoupling. On the other hand, a decoupling timescale approaching infinity implies no decoupling at all. For our fiducial model, we adopt $\tau_{\text{dec}} = 1.5 \times 10^4$ yr, which is the same as that used in Cassen (1996).

In our simulations, we choose a disc evolution timescale...
of \( t_e = 2.625 \times 10^4 \) yr and a dust decoupling timescale \( t_{\text{dec}} = 1.5 \times 10^7 \) yr as our typical case. These values match the typical case used in Cassen (1996). All these models and the parameters we used for them are shown in Table 2.

5.2 Model 2: Time-dependent chemical equilibrium model

In the second model, we use the GRAINS code to calculate the chemical equilibrium dynamically throughout the evolution of the disc.

\[
\frac{d\Sigma_i}{dt} = \varepsilon_i \Omega \Sigma_i
\]

(11)
to calculate the surface densities of the decoupled dust as described in Section 5.1. Here \( \Sigma_i \) is the surface density of element \( i \) in the advecting dust. \( \Sigma_i \) changes smoothly from 0 to values that larger than 0 as the temperature decreases from a high value to values less than the condensation temperature where the elements begin to condense, see Table 1 and Figure 4. This is different from Equation (9), used in the \( T_{50} \) calculations, where \( \Sigma_i \) jumps from 0 to a value that equals the surface density of the gas when the temperature becomes less than \( T_{50} \). Note that the condensation temperature for an element (where the element begins to condense) is higher than \( T_{50} \) (where half of the element has already condensed, see Table 1). We use the same formula to calculate the decoupling as Cassen (1996). However, since we calculate the chemical equilibrium of the system, the process is quite different from his work.

To save computational time, we do not calculate the chemical equilibrium at every timestep of the disc evolution. Rather, we calculate the chemical equilibrium everywhere in the disc whenever the midplane temperature at 1.8 AU changes by 1 K. The reason we choose this radius and this temperature step is that the temperature steps at this radius are small enough to limit the size of the temperature steps at all other radii that we consider.

To verify that these choices do not affect our results, we test the convergence of the condensation results by running several simulations where we fix the temperature step at 1.8 AU to be several values in the range between 1 and 100 K. Figure 7 shows that if the temperature step is less than or equal to 10 K, the differences between the results are less than 1%. Consequently, we do not need to use a temperature step that is smaller than 1 K (which yields errors at a level near \( 10^{-3} \)) to ensure the accuracy of our simulations and we adopt this temperature step throughout our work.

6 RESULTS

We now compare the results of our three models. We also examine the effects of different disc evolution timescales and decoupling timescales on our results.

6.1 Relative elemental abundances from the new 50% condensation temperatures

The results of MC (the historical Cassen (1996) model) are in Figure 8 (a). It shows the \( R_i \) at 1, 2, 3, and 4 AU along with the observed abundances of CM, CO, and CV condrites for 13 elements. At 1, 2, and 3 AU, the \( R_i \) decline with decreasing \( T_{50} \). This decline arises because the temperatures at these radii start above \( T_{50} \) for Si (1316 K) and falls over time. At 4 AU, the \( R_i \) are almost unity for elements with \( T_{50} \) higher than \( \sim 1000 \) K (around the \( T_{50} \) for Na) and then decreases because the initial temperature here is \( \sim 1000 \) K and all elements with \( T_{50} \) higher than this value condense simultaneously. For elements with \( T_{50} \) lower than \( \sim 1000 \) K, they condense later and therefore have a lower relative abundance.

Figure 8 (b) shows \( R_i \) by using updated \( T_{50} \) calculated from the GRAINS code (M1G1). There are more refractory elements in Figure 8 (b) than in Figure 8 (a) as the GRAINS Code considers more elements. The general trends at 1 and 2 AU are similar to those in Figure 8 (a). At 3 AU, \( R_i \) for elements \( T_{50} \) higher than Ca (1500 K) are almost the same value because the initial temperature at this radius is near \( T_{50} \) for Ca and these elements begin condensing simultaneously. Because the temperature interior to 4 AU decreases with time, the value of \( R_i \) for an element is determined by the initial value of temperature at a given radius. If the initial temperature at a radius is lower than the \( T_{50} \) for Si (1316 K), \( R_i \) will be 1. If the initial temperature is higher than \( T_{50} \) for the most refractory element, \( R_i \) will decrease with decreasing \( T_{50} \).

6.2 Relative abundances from the full condensation sequence

We now consider our second new model where we follow the entire condensation sequence of the dust assuming chemical equilibrium throughout the evolution of the disc. The gaseous phases and advecting dust flow with the gas while the decoupled dust remains where it condenses.

The resulting \( R_i \) for times at \( t = 2.5 \ t_e \) and \( t = 5 \ t_e \) are...
shown in Figure 11 (M2G1). The general trends at $t = 5 t_\text{c}$ are consistent with the observations, i.e., the values are higher than that of Si for elements with higher $T_\text{50}$ (refractory elements), while the values are lower for volatile elements. Relative elemental abundances, $R_i$, are different at different radii. If the temperature decreases from a high value that is larger than $T_\text{50}$ for Si (1316 K, at 1, 2, and 3 AU), the elements with high $T_\text{50}$ condense first and there will be more refractory elements in the condensed materials and $R_i$ is above unity. At 4 AU, the temperature is less than the $T_\text{50}$ for Si (1316 K), so the refractory elements condense along with the Si and the values are generally equal. The difference between $R_i$ and unity mainly comes from the difference of the composition of CI (Asplund, Grevesse & Sauval 2005) and that of the Solar atmosphere (Lodders 2003).

On the other hand, if the temperatures are high, the $R_i$ is low for volatile elements because the volatile elements condense later. The relative elemental abundances are higher for refractory elements and lower for volatile elements at $t = 2.5 t_\text{c}$ than that at $t = 5 t_\text{c}$ at 1, 2, and 3 AU because the temperature is high during the early evolution of the disc. For example, at $t = 2.5 t_\text{c}$ and at 1 AU, $t = 1213$ K and Si just begins to condense. Thus, the amount of Si is low and $R_i$ is correspondingly high for refractory elements. The volatile elements have even less time to condense, so $R_i$ is low. The relative elemental abundances at 3 AU most closely match the measured abundances of the chondrites (CM, CO, and CV). Since we do not know where these chondrites formed, our results suggest that they may form at the present-day location of the asteroid belt (Tedesco & Desert 2002).

### 6.3 Comparison of the three nominal models

In Figure 10 we show the evolution of $R_i$ for Al, Si, S, Os, and Au at 3 AU for our two new models. Al and Os are both refractory elements with $T_\text{50}$ for Al (1654 K) and Os (1812 K) both higher than that for Si (1316 K). Thus, their $R_i$ decrease over time as more Si condenses. The final ratios calculated from the chemical equilibrium are slightly larger than those calculated using $T_\text{50}$.

Both S and Au are more volatile with their $T_\text{50}$s being lower than that for Si: S (669 K) and Au (1196 K). Thus, their $R_i$ increases over time from 0 to their final values. Note that the dust begins to condense earlier in the chemical equilibrium calculation than it does in the $T_\text{50}$ calculations. The ratios of the final values of $R_i$ for these elements are similar between the two models. However, the approximation from the 50% condensation temperature systematically overestimates the volatile abundance (3% for S and 1% for Au) while it systematically underestimates the refractory abundances (2% each for Al and Os).

Figure 11 shows that $R_i$ calculated from chemical equilibrium is higher than that calculated from the $T_\text{50}$ model at 1, 2, and 3 AU for refractory elements while it is lower for volatile elements. At 4 AU, $R_i$ is almost of the same value for elements with $T_\text{50}$ higher than that for Cu (1100 K).

### 6.4 Different decoupling timescales and disc evolution timescales

To illustrate the conditions under which our simulations can reproduce the chondrite abundances, as well as the main factors that may affect other scenarios, we look at the effects of changes to the disc evolution timescale and decoupling timescale on the relative abundances. We first change the decoupling timescale, $t_\text{dec}$, to be an order-of-magnitude longer than the typical case ($1.5 \times 10^5$ yr M2G2, Figure 12 (a)). We find that these results are almost the same as those for the typical case. This agreement arises because the decoupling timescale is very long and there is more material in the gas and advecting dust. This material flows with the gas and leaves behind the same relative abundances of decoupled dust. Thus, while less material condenses overall, the relative amount of the elements in the decoupled dust stays almost the same. This result does not change when we use even longer decoupling timescales.

We also change the decoupling timescales to be an order-of-magnitude shorter than the typical timescale (M2G3, $1.5 \times 10^3$ yr). Figure 12 (b) shows the corresponding abundances at different radii. These results are quite different from the typical case as there is less advecting dust to transport throughout the disc. At large distances, with the disc model we are using, the disc material flows outward (Figure 8 (d)). The more refractory elements in the inner disc will decouple and enrich the outer regions with more volatile elements. This effect can be seen in the peaks of the abundances of different elements (e.g., at 3 and 4 AU).

Compared to Figure 9, the abundances at 4 AU peak at Copper, with a $T_\text{50}$ of 1100 K. The more refractory elements have lower $R_i$ because they condense and quickly decouple in the inner regions and do not flow out this far. The most refractory elements at 4 AU have the lowest $R_i$. Cu has the largest abundance because it condenses and decouples at the beginning of the simulation and additional copper is advected into that region from the inner disc (where it is too hot for copper to condense) while the more refractory elements remain behind. At 3 AU, a similar effect happens with Calcium. The more refractory elements also have lower

| Time-dependent chemical equilibrium model | (M2) |
|-----------------------------------------|------|
| $t_\text{dec/yr}$ Typical values Group 3 Typical values Group 2 Group 3 Group 4 |
| $t_\text{c/yr}$ Typical values Group 3 Typical values Group 2 Group 3 Group 4 |

### Table 2. Different models and disc evolution and dust decoupling timescales.

| Timescales | Historical model (MC) | Models with new $T_\text{50}$ (M1) | Time-dependent chemical equilibrium model (M2) |
|------------|----------------------|----------------------------------|-----------------------------------------------|
| $t_\text{dec/yr}$ | Typical values (MC) | Typical values (M1G1) | Typical values (M1G3) |
| $t_\text{c/yr}$ | Typical values (MC) | Typical values (M2G1) | Typical values (M2G2) |
| $t_\text{dec/yr}$ | Typical values (MC) | Typical values (M4G1) | Typical values (M4G2) |
| $t_\text{c/yr}$ | Typical values (MC) | Typical values (M4G3) | Typical values (M4G4) |
R_i while the more volatile elements have higher R_i for elements with T_{50} larger than that for Ca (1500 K).

The trend at 2 AU is similar to that of the typical case, i.e., the more refractory elements have higher abundances. The difference is that they are more abundant than the typical case as shown in Figure 9. The reason for the increased abundance at 2 AU is the same as what we saw at 3 and 4 AU. However, we note that with our disc model, the direction of the disc flow changes as the disc evolves (see Figure 8(d)). Thus, later in the evolution of the dust in this region,
the arriving material has had a different history and is depleted in refractory elements and can be slightly enriched in volatiles. This effect can be seen most prominently at 1 AU where all of the material arrives from the outer regions.

At 1 AU, when the decoupling time is very short, all of the material that arrives from the outer regions will be depleted refractory elements. At the same time, the volatile elements (including silicon) will flow into the region. This additional material will yield lower refractory abundances overall and will produce a slight enrichment in the abundances of the volatiles. This effect can be seen in Figure 12 but is not seen in our primary result for this work (Figure 9).

To see how the disc evolution timescale affects $R_i$, we change both the decoupling timescale and the disc evolution timescale to be two orders-of-magnitude longer than the typical case while keeping the ratio the same (M2G4). With the disc evolution timescale two orders-of-magnitude longer than the typical case, the accretion rate from the disc to the central star reduces to two orders-of-magnitude shorter than the typical case while keeping the ratio the same (M2G4). With the longer decoupling time there is a consistent trend in the relative abundances with distance. With the short decoupling time we observe peaks in the abundances where the initial temperature in the disc correlates with the condensation temperature of the element at that particular radial distance. Also, with short condensation times, the innermost region (where the gas flows toward the star rather than away) the refractory elements are depleted somewhat as the incoming gas from more distant regions contains a higher proportion of volatile elements (see text for details).

Figure 11. Equilibrium vs 50% condensation models (M2G1 vs M1G1): Comparison of $R_i$ calculated from the two new models. The chemical equilibrium model (M2G1, solid lines) and the fixed $T_{90}$ (M1G1, short dotted lines) for the elements in the evolving discs are shown.

Figure 12. Effects of changes to the decoupling timescale (M2G2 and M2G3): These panels show the effect of changing the decoupling timescale of the dust relative to the disc evolution timescale. Values of $R_i$ at different radii and at time $t = 5$ $t_{\text{e}}$ ($t_{\text{e}} = 2.625 \times 10^5$ yr) calculated from the evolution of disc and using the GRAINS code. The decoupling timescales here are (a) $1.5 \times 10^4$ yr (M2G2) and (b) $1.5 \times 10^3$ yr (M2G3), which are one order of magnitude longer or shorter than that in the typical case respectively. The elements are ordered from high to low (see text for details).
evolution timescale and the dust decoupling timescale (i.e., the planetesimal formation timescale) is that there will be peaks in the radial distribution of abundances of different elements that depend upon their condensation temperatures. If planetesimals form quickly, then the more refractory elements will not flow with the gas, and regions fed by the warmer parts of the disc will be somewhat depleted in those elements. On the other hand, if planetesimals form more slowly (a large decoupling timescale), then the advecting refractory materials will enrich neighboring parts of the disc. Definitive statements about the consequences of this effect will require a more realistic disc model.

7 DISCUSSION

7.1 Elemental evolution of decoupled dust

In Figure 14 (a), we show how silicon and calcium in the decoupled dust evolve with time. The silicon first condenses at locations between 3.2–5.8 AU. Inside ~ 3.2 AU, the temperature of the disc is too high for silicon to condense. Outside ~ 5.8 AU, the gas surface density is too low for silicon to condense. As time goes on, the condensation region expands both inward and outward.

The condensation front moves inward as the temperature of the inner region decreases and the material can condense. The condensation area expands outwards as the gas surface density increases due to viscosity and the outward flow of disc material. The general trend of the evolution of calcium is similar to that of silicon except the maximum surface density and the inner and outer boundaries of the condensed region. The different maximum surface densities and outer boundaries are determined by the different gas surface densities of the elements. The inner boundaries are correlated with the $T_{50}$ for the elements.

Figure 14 (b) shows the abundances of Ca, Mg, Fe, and S as a function of radius and time. Calcium has the highest condensation temperature (1669 K) and the highest $T_{50}$
(1500 K), both of which are larger than that of silicon (1478 K condensation and 1316 K \( T_{50} \)). Calcium is more abundant at the inner region of the disc and decreases sharply to match the abundance of silicon at the point where silicon also condenses. The condensation temperature of magnesium (1385 K) is lower than that of silicon while its \( T_{50} \) (1336 K) is slightly higher. Consequently, its abundance stays essentially near unity—tracking the abundance of silicon everywhere except at the inward-moving condensation front. Iron has similar relative condensation temperature to silicon (1360 K) and \( T_{50} \) (1335 K) and its \( R_i \) shows a trend similar to magnesium. The condensation temperature (711 K) and \( T_{50} \) (669 K) of sulfur are the lowest. Its \( R_i \) increases with radius when \( R > 1 \) AU. \( R_i \) for all the four elements are around 1 at \( R > 5 \) AU due to the low temperatures of the disc. The abundances of the refractory elements decrease with time (Ca, Mg, Fe) while those of the volatile elements (S) increase with time (See also Figure 10).

### 7.2 Comparison with the observations

To compare our results from the three condensation models to the element compositions of the CM, CO, and CV condrites we adopt the decoupling timescale to be \( 1.5 \times 10^4 \) yr and disc evolution timescale \( t_e = 2.625 \times 10^4 \) yr (both values adopted from the historical model of Cassen (1998)). The historical model reproduces the general trends for volatile elements of the condrites as do our two new models. However, the relative abundances are different at different radii. Our full condensation model most closely matches the observed abundances at 3 AU. This fact may indicate that those condrites come from the present-day asteroid belt between Mars and Jupiter.

The more refractory elements of CM, CO, and CV condrites with \( T_{50} \) higher than that for Ti (1583 K) have lower relative abundance (Figure 9). With the standard decoupling and disc evolution timescales, the quick depletion of the refractory elements affects the transfer of elements to different radii. This effect can explain the relatively low relative abundances of the most refractory elements. For example, the three most refractory elements Re, Os, and W do not have the largest abundances in the condrites.

The average values of the relative abundance for refractory elements for Mercury, Venus, Earth, and Mars are 1.80, 1.17, 1.32, and 1.02, respectively. For volatile elements, the values are 0.0877, 0.274, 0.105, and 0.381 (See Figure 1). Generally, the values are high at small orbital distances for refractory elements (except Venus) and low at small orbital distance for volatile elements. This observation is consistent with the results shown in Figure 9 that the relative abundance is high at small radius for refractory elements while the relative abundance is low at small radius for volatile elements.

Figure 12(b) shows that the relative abundance for refractory elements can decrease toward small radii while increasing slightly for volatile elements. A short decoupling timescale may explain the slightly lower refractory abundances of Venus compared to the Earth. The surface density and the temperature in the inner region of the model are high compared to a more realistic disc model. Therefore, if we get the same relative abundance for the terrestrial planets in our disc, the semimajor axes will be larger than the actual locations of the terrestrial planets in a real disc. Addressing this problem, using a more realistic disc model (Li & Sui 2017), lies beyond the scope of the present work.

### 8 CONCLUSIONS

To explain the observations that the chondrites (CM, CO, and CV) and terrestrial planets are rich in refractory elements and poor in volatile elements, we calculate the condensation of elements in the evolving disc. Three condensation models are adopted in the paper. In the first two models we use \( T_{50} \) as a typical value below which the elements will condense. In the third model, we calculate the chemical equilibrium of 33 elements by minimizing the Gibbs free energy of the system at each radius and specific time steps in the evolving disc.

Compared with previous works, our models have improvements in 1) using chemical equilibrium calculation to model the condensation of the elements rather than fixed \( T_{50} \), 2) significantly increasing the number of elements used in the calculation, and 3) embedding the elements in a dynamically and thermally evolving protoplanetary disc rather than choosing one or several snapshots in the evolving discs.

From our results we draw the following conclusions:

For each element, the condensation front expands inward and outward from its initial condensation region. The inner edge of this region advances because of the decreasing temperature with time. The outer edge of the region retreats because of the outward movement of the gas in the disc, which increases the disc surface density.

The relative abundances of the condensed elements in the disc vary with time and distance—decreasing with time and distance for refractory elements and increasing with time and distance for volatile elements within ~ 3 AU. The resulting condensed materials are rich in refractory elements and poor in volatile elements within ~ 3 AU. Comparing our calculated \( R_i \) with those measured in the chondrites (CM, CO, and CV) shows that our results at 3 AU most closely match the observed abundances.

Approximating the condensation process with a fixed \( T_{50} \) produces results that are similar to those that arise in the full chemical equilibrium model. However, there are systematic differences from refractory to volatile elements. The relative elemental abundance, \( R_i \), calculated from the chemical equilibrium is higher for refractory elements and lower for volatile elements within 3 AU. (That is, the 50% condensation model will underpredict refractories and will overpredict volatiles.) Nevertheless, depending upon the circumstances, the \( T_{50} \) model may be sufficient for one’s purposes. These systematic differences can be large as 10% and may become more important with further refinements of the disc model.

The relative abundances do not change significantly when the decoupling timescale is longer than or similar to the disc evolution timescale. Rather, the surface density of the material is lessened because the advecting dust drifts out of the region of interest.

If the decoupling time is short, there will be peaks in the abundance distribution as a function of the condensation temperature. The relative abundance of refractory elements can be diminished at small semimajor axis because the refractory elements from more distant regions would decouple
and remain while the volatile elements will flow toward the
star, diluting the refractory elements. This may explain the
estimated lower abundance of refractory elements in Venus
compared with Earth.
When the initial temperature in the disc is high, the abun-
dances of refractory elements is above unity, while it is low
for volatile elements because the refractory elements con-
dense and decouple while the Silicon flows with the gas.
When the initial temperature is low, the refractory abund-
dances are around unity since they condense at the same
time as Silicon. Thus, the relative elemental abundance, \( R_i \),
is affected by the temperature history of the disc.

As we use more elements, it may be possible to explain
the compositions of meteorites and planets in more detail.
By including the effects of the transport of the elements in
the disc, our results can provide more information on the
history of the dust within the disc and may yield better
estimates for the dust in planet forming discs generally. We
can explain both the broad trends of the compositions as a
function of \( T_{50} \) and the cases that do not follow these trends.
We notice that the thermal history can have a significant
effect on the results. By including this aspect of the evolution
of the disc we can improve our understanding of the origins
of the composition of the meteorites and planets.

There are some limitations to our current disc model.
The surface density and the temperature in the inner region
of the disc in this model are high compared to a more realistic
disc model. Using a more realistic disc model will result
in a smaller semimajor axes for the formation location of
the planetesmals and the planets. Due to the relative low
initial temperature in the disc, it will also affect the relative
elemental abundance. Incorporating an improved disc model
is left for future work.

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