Presolar grain dynamics: creating nucleosynthetic variations through a combination of drag and viscous evolution

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ABSTRACT

Meteoritic studies of solar system objects show evidence of nucleosynthetic heterogeneities that are inherited from small presolar grains (< 10 μm) formed in stellar environments external to our own. The initial distribution and subsequent evolution of these grains are currently unconstrained. Using 3D, gas-dust simulations, we find that isotopic variations on the order of those observed in the solar system can be generated and maintained by drag and viscosity. Small grains are dragged radially outwards without size/density sorting by viscous expansion and backreaction, enriching the outer disc with presolar grains. Meanwhile large aggregates composed primarily of silicates drift radially inwards due to drag, further enriching the relative portion of presolar grains in the outer disc and diluting the inner disc. The late accumulation of enriched aggregates outside Jupiter could explain some of the isotopic variations observed in solar system bodies, such as the enrichment of supernovae derived material in carbonaceous chondrites. We also see evidence for isotopic variations in the inner disc that may hold implications for enstatite and ordinary chondrites that formed closer to the Sun. Initial heterogeneities in the presolar grain distribution that are not continuously reinforced are dispersed by diffusion, radial surface flows, and/or planetary interactions over the entire lifetime of the disc. For younger, more massive discs we expect turbulent diffusion to be even more homogenising, suggesting that dust evolution played a more central role in forming the isotopic anomalies in the solar system than originally thought.

Key words: protoplanetary discs — circumstellar matter — planetary systems — stars: pre-main sequence — hydrodynamics — meteorites, meteors, meteoroids

1 INTRODUCTION

Meteorites originate from planets and other debris that formed shortly after the Sun and, as such, provide a valuable fossil record of the events that transpired in the protosolar neighbourhood. Sample return missions from different objects in the solar system have (e.g. Wood et al. 1970; Smith et al. 1970; Brownlee et al. 2006; Fujiwara et al. 2006) and will continue (Tachibana et al. 2014; Lauretta et al. 2019) to provide a wealth of new information about their origin and structure. Still, the most varied and abundant source of information comes from material intercepted by the Earth itself in the form of interplanetary dust particles, micrometeorites, and meteorites (e.g. Dodd 1981; Papike et al. 1998; Bradley 2003; Hutchison 2006; Lauretta & McSween 2006; Genge et al. 2008).

An important property of meteorites is that they contain isotopic anomalies relative to Earth (Black & Pepin 1969; Black 1972) that can be linked to interstellar origins (Ming & Anders 1988; Amari et al. 1990). Of particular interest are the isotopic abundances of heavier elements (including Ca, Ti, Cr, Ni, Sr, Zr, Mo, Ru, Pd, Ba, Nd, Sm and W; see Qin & Carlson 2016; Mezger et al. 2020), which are produced in different nucleosynthetic production sites, such as asymptotic giant branch stars (AGB), supernovae, and neutron-star mergers. The processes include, among others, slow neutron capture (s-process; e.g. Pignatari et al. 2010; Stancliffe et al. 2011; Bisterzo et al. 2011; Karakas et al. 2012; Frischknecht et al. 2012), rapid neutron capture (r-process; e.g. Freiburghaus et al. 1999; Goriely et al. 2011), and/or the p-process (p-for proton, sometimes referred to as the γ-process due to the likely role of photodisintegration; e.g. Rauscher et al. 2002; Arnould & Goriely 2003; Travaglio et al. 2018). In each case, the isotopic fingerprint created by local nucleosynthetic processes is imprinted on the refractory condensates that were ejected into the interstellar medium (ISM) and ultimately inherited by the protosolar molecular cloud.

In addition to providing vital information about the environment in which the Sun formed, presolar grains are perhaps the most direct way of tracing the genetic and dynamical history of solids

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in the solar system. Their isotopic fingerprints (e.g. Lewis et al. 1987; Bernatowicz et al. 1987; Nicollussi et al. 1997, 1998a,b; Nittler 2003; Zinner et al. 2007; Zinner 2014) are responsible for a number of isotopic variations observed in bulk samples of primitive chondrites, some of which (e.g. Ti and Cr) display a clear dichotomy between non-carbonaceous chondrites (NC) formed in the inner solar system and the carbonaceous chondrites (CC) that formed further out (Trinquier et al. 2007; Leya et al. 2008; Ebert et al. 2018). It is still unclear whether this division reflects an inherited heterogeneity from the Sun’s nascent molecular cloud (Clayton 1982; Dauphas et al. 2002, 2004; Nanne et al. 2019; Ek et al. 2020), fractionation of material during infall (Van Kooten et al. 2016), subsequent evolution within the circumstellar disc due to thermal processing (Trinquier et al. 2009; Burkhardt et al. 2012; Paton et al. 2013; Schiller et al. 2015; Akram et al. 2015; Poole et al. 2017; Ek et al. 2020), dynamical sorting brought on by growth and aerodynamic drag (Pignatel et al. 2017, 2019), or interactions with early Jupiter (Alibert et al. 2018). Determining which mechanism (or combination thereof) is responsible for the nucleosynthetic heterogeneity in chondrites may therefore provide essential information about the history of the early solar system.

The distinct isotopic fingerprints carried by presolar grains are responsible for certain nucleosynthetic signatures observed in bulk samples of meteorites from asteroids and planets. To understand how these signatures vary as a function of location in the solar system, it is required to track the presolar grain populations through the many dust processes that take place in discs1: coagulation (Weidenreich 1980; Dullemond & Dominik 2005; Ormel et al. 2007), fragmentation (Blum & Münch 1993; Schäfer et al. 2007; Birnstiel et al. 2009), erosion (Schräpler & Blum 2011; Krijt et al. 2016), and sublimation (Dullemond et al. 2001; Kobayashi et al. 2012). Simulating these processes for mixtures of compositionally unique dust populations is still challenging for current models, particularly given the dependence of the above processes on the detailed chemical makeup of the dust (Blum & Wurm 2008) and, potentially, the properties of the surrounding gas (e.g. Isella & Natta 2005).

However, even before tackling the more difficult problem of size evolution, there is still much that we can learn from simulating the isotopic signatures that are produced when presolar grains are evolved independently from other grain types. Although presolar grains are tightly coupled to the gas on account of their small sizes (< 10 μm e.g. Yokoyama & Walker 2016), their dynamics is far from simple. For example, the cumulative effect of viscous stresses (e.g. Shakura & Sunyaev 1973; Lynden-Bell & Pringle 1974), diffusion (e.g. Schräpler & Henning 2004; Johansen & Klahr 2005), backreaction from multiple grain sizes (Takeuchi & Lin 2002; Bai & Stone 2010; D’ipierro et al. 2018), interactions with a planet (e.g. Kley & Nelson 2012), etc. can lead to some counterintuitive results that have already grown to mm–cm sized objects. We measure the effect of backreaction on grains by comparing select single-grain simulations with the same physical properties and initial conditions as several of our dust phases in multi-grain simulations. We similarly assess the isolating effects of a disc gap by comparing models with and without a Jupiter-mass planet initialised at various locations in the disc. Finally, taking the dust surface densities from our simulations, we use mass-balance equations to calculate isotopic ratios for 54Cr, 96Zr, and 50Ti as a function of disc radius and compare these against the meteorite record in the solar system. Given that the forces driving evolution in our simulations (i.e. drag and viscosity) are generic and present in almost all protoplanetary discs, we expect the resulting isotopic variations to be robust.

The structure of the paper is as follows. In Section 2 we outline the databases used to obtain our presolar grain data, the discretisation process for our three dust populations, the setup and initial conditions for our simulations, and our method for calculating isotopic compositions. In Section 3 we present our simulation results, including a breakdown of the dynamical contributions from drag and viscosity, and the isotopic variations that we calculated from the final dust surface densities. In Section 4 we discuss the origin of the isotopic variations and how these variations may change under different physical conditions. For added physical insight, we conclude by comparing our results to meteorite data from the solar system. A summary of our main conclusions is given in Section 5.

2 METHODS
2.1 Presolar grain laboratory data

We obtained our presolar grain sizes from the online Presolar Grain Database (Hynes & Gyngard 2009), which is a collection of published presolar grain data in the literature. While there are many types of presolar grains, we focussed only on two: the abundant silicon carbide (SiC) grains and presolar oxides (Ox). Furthermore, many grains within these two subcategories do not contain size information and have therefore been omitted from our data set. In particular, out of 732 presolar oxides, only 67 have size information and can be used to define a size distribution. Similarly, size information is available for 5102 out of 11042 SiC grains2. We assume a density of \( \rho_{\text{SiC}} = 3.16 \text{ g cm}^{-3} \) for presolar SiC grains. Because oxide grains are composed of different phases (e.g. corundum, hibonite, or spinel), we defined the density of this population as a weighted average of these phases: \( \rho_{\text{Ox}} = 3.93 \text{ g cm}^{-3} \). All densities were obtained from Barthelmy (2012).

In the context of our simulations, we shall hereafter use the term ‘presolar grains’ to refer exclusively to SiC and Ox grain types and refer to all remaining dust grains (regardless of origin) as solar system silicates (SSI). These are the three unique dust populations mentioned in Section 1 that we evolved in our simulations.

1 Similar processing takes place prior to or during infall (Sittner et al. 1999; Hirashita & Yan 2009; Ormel et al. 2009) and may also need to be considered.

2 Since performing our simulations, another 448 SiC grains with size information have been added to the database (Stephan et al. 2020), but the change to our derived size-distribution in Section 2.2.2 is negligible.
2.2 Discretising the grain-size distributions

We formulated an analytic grain-size distribution for each species that can be arbitrarily discretised and integrated to obtain the optimal number of grain sizes and associated dust masses for our simulations. Although the data from Section 2.1 was already discretised, using the analytic distributions gave us the freedom to choose the number of simulated grain sizes in each species without increasing runtimes and file sizes. It also provided a globally consistent method for fixing the dust mass that could be applied to both presolar and silicate grains alike.

2.2.1 Silicate grains

The number density \( n(s) \) for silicate grains canonically follows a truncated power-law (e.g. Draine 2006):

\[
\frac{dn}{ds} = A \left( \frac{\rho_{d,\text{Si}}}{s_{\text{max}}^{1/n}} \right) \left( \frac{s}{s_{\text{max}}} \right)^{-\gamma} \quad \text{for} \quad s_{\text{min}} \leq s \leq s_{\text{max}},
\]

where \( A \) is a dimensionless normalisation constant, \( \rho_{d,\text{Si}} \) is the local silicate dust density in the disc, and \( m(s) \) is the mass of an individual grain as a function of grain size. The distribution typically has a MRN power-law index of \( \gamma = 3.5 \) taken from ISM observations (Mathis et al. 1977) with a minimum and maximum grain size, \( s_{\text{min}} \) and \( s_{\text{max}} \), respectively. Alternatively, we chose to model the dust-to-gas ratio \( \epsilon \) (equivalent to modelling the mass distribution), which is related to the number density by

\[
\frac{de}{ds} = \frac{m(s) \, dn}{\rho_g} \propto \epsilon |s|^{-3},
\]

where \( \rho_g \) is the local gas density in the disc. The proportionality relation comes from assuming the dust grains are spherical (i.e. \( m = 4\pi \rho_{\text{grain}} s^3/3 \)) with a uniform intrinsic density \( \rho_{\text{grain}} \) and by replacing \( \rho_d,\text{Si}/\rho_g \) by the total silicate dust-to-gas ratio \( \epsilon \).

We used Equation (2) to discretise our silicate grains into \( N_{\text{Si}} = 10 \) bins with logarithmically-even widths of \( \Delta \log s = \frac{\log_{10}(s_{\text{max}}/s_{\text{min}})}{N_{\text{Si}} - 1} \) spanning \( s_{\text{min}} = 0.1 \, \mu m \) to \( s_{\text{max}} = 1 \, \text{cm} \). We chose the simulated grain size for each bin to be the logarithmic midpoint, or equivalently, the square root of the product of the cell’s endpoints — thereby skewing the representative grain size for each cell towards the smaller, more numerous dust grains in each bin. Finally, we set the intrinsic grain density to \( \rho_d,\text{Si} = 3 \, \text{g cm}^{-3} \) and normalised the integrated distribution so as to maintain a combined total dust-to-gas ratio of \( \epsilon = 0.01 \). After accounting for the presolar grain populations (see the following section), the initial silicate dust-to-gas ratio we assumed for the disc was \( \epsilon_{\text{Si}} = 9.9987 \times 10^{-3} \).

2.2.2 Oxide and silicon carbide grains

In order to discretise and assign dust masses to the presolar grain populations in a manner consistent with Section 2.2.1, we needed analytic functions for each distribution. As a preliminary step to making the fitting easier, we rebinned the raw data into larger contiguous size bins\(^3\) using the so-called Scott method (Scott 1979), which selects the ‘optimal’ bin width by asymptotically minimising

\[
\epsilon = 0.01.
\]

The combination of the \( s^3 \) mass dependence with the GEV probability density function is not integrable in terms of elementary functions and must be done numerically.

\[^3\] There is always some arbitrariness associated with binning data (see He & Meeden 1997). For example, we found that the binning method can influence the location of the peak distribution by up to \(-0.5 \, \mu m \). However, these fluctuations turn out to be of minor importance since we do not see any significant size/density sorting between presolar grains within the disc (e.g. see Figure 3).
Figure 1. Normalised probability densities as a function of grain size for the oxide (blue), SiC (orange), and silicate (yellow) grains used in this study. The semi-transparent histograms show the binned presolar grain abundances that we used to fit the GEV distribution functions. The silicate grains follow the usual MRN-like power-law distribution from Equation (1). Open symbols indicate the representative (i.e. simulated) grain size from each size/mass bin while filled circles mark the edges of the corresponding bins.

Table 2. The grain size $s_j$ and dust-to-gas ratio $\varepsilon_j$ for the 17 dust species in our fiducial setup with $\varepsilon = 0.01$. The total dust-to-gas ratio for each population is given at the bottom of each section, including the total solid-to-gas ratio for the disc (bottom row). When accounting for the partial incorporation of presolar grains into larger silicate grains, the dust-to-gas ratio of the unincorporated grains (dynamical mass) is obtained by multiplying $\varepsilon_j$ by the appropriate scaling factor $f_{SSi}$, $f_{SiC}$, or $f_{Ox}$ (see Section 2.2.3). The final column contains the minimum and maximum grain sizes of the mass distribution and the intrinsic grain density for each grain type.

| Type  | $s_j$ [cm] | $\varepsilon_j$ | Population properties |
|-------|------------|-----------------|-----------------------|
| Ox:   | 1 1.35 x 10^{-5} | 1.4727 x 10^{-5} | $s_{\text{min}} = 0.100 \mu m$ |
|       | 2 2.45 x 10^{-5} | 3.4113 x 10^{-7} | $s_{\text{max}} = 0.600 \mu m$ |
|       | 3 4.45 x 10^{-5} | 6.4401 x 10^{-7} | $\rho_{\text{grain}} = 3.160 \text{ g cm}^{-3}$ |
|       | 4 9.9987 x 10^{-3} | 9.9987 x 10^{-3} |  |
| SiC:  | 4 3.56 x 10^{-5} | 8.1962 x 10^{-5} | $s_{\text{min}} = 0.250 \mu m$ |
|       | 5 7.22 x 10^{-5} | 3.0145 x 10^{-7} | $s_{\text{max}} = 4.225 \mu m$ |
|       | 6 1.46 x 10^{-4} | 1.3128 x 10^{-7} | $\rho_{\text{grain}} = 3.930 \text{ g cm}^{-3}$ |
|       | 7 2.97 x 10^{-4} | 1.8771 x 10^{-7} |  |
|       | 3.4995 x 10^{-3} | 3.4995 x 10^{-3} |  |
| SiS:  | 8 1.78 x 10^{-3} | 2.4686 x 10^{-3} | $s_{\text{min}} = 0.100 \mu m$ |
|       | 9 5.62 x 10^{-5} | 4.3899 x 10^{-3} | $s_{\text{max}} = 1.000 \mu m$ |
|       | 10 1.78 x 10^{-3} | 7.8064 x 10^{-4} | $\rho_{\text{grain}} = 3.000 \text{ g cm}^{-3}$ |
|       | 11 5.62 x 10^{-4} | 1.3882 x 10^{-3} |  |
|       | 12 1.78 x 10^{-3} | 2.4686 x 10^{-4} |  |
|       | 13 5.62 x 10^{-3} | 4.3899 x 10^{-4} |  |
|       | 14 1.78 x 10^{-2} | 7.8064 x 10^{-4} |  |
|       | 15 5.62 x 10^{-2} | 1.3882 x 10^{-1} |  |
|       | 16 1.78 x 10^{-1} | 2.4686 x 10^{-3} |  |
|       | 17 5.62 x 10^{-1} | 4.3899 x 10^{-3} |  |
|       | 9.9987 x 10^{-3} | 9.9987 x 10^{-3} |  |
|       | 1.0000 x 10^{-2} | 1.0000 x 10^{-2} |  |

The above formalism assumes all of the presolar grains are in what we call a dynamical state, free to evolve independently of other grain types. This is akin to inheriting all of the presolar grains in the disc at once. More realistically, we would expect presolar grains to be inherited over a prolonged period of time and that a significant portion of the total presolar grain mass in the disc would be in an aggregate state, having been swept up by larger aggregates during prior evolution. Given the low dust-to-gas ratios of presolar grains in Table 2, the probability of forming pure presolar aggregates is negligible and the finite size distribution can account for the rare cases in which they do collide and grow (fragmentation of such small, compact grains can be neglected). In what follows we will refer to the presolar mass in free-floating grains that dynamically evolve independently of the silicates as the dynamical mass and the presolar mass contained within silicate aggregates as the aggregate mass.

We assume the presolar dynamical mass and similarly sized silicate grains are either continuously resupplied by fragmentation and/or by infall\(^5\) from the envelope, although we do not model these processes in our simulations. As a result, the ratio of dynamical mass to the aggregate mass is left as a free parameter in our model. This ambiguity propagates through to the isotopic anomalies but only affects the overall amplitude of the variations because the presolar grains are passive in nature (i.e. they do not strongly affect the dynamics of the simulation on account of their tight coupling with the gas and their small dust-to-gas ratios). An important consequence of being passive is that, as long as the total dust-to-gas ratio of each dust population is preserved, shifting presolar dust mass between the dynamical and aggregate mass reservoirs represents a small perturbation to the disc that is hidden within the numerical noise of the simulation.

In lieu of exploring different dynamical masses by running multiple sets of simulations with nearly identical particle distributions/dynamics, we ran one set of simulations with all presolar grains in the dynamical mass (i.e. the dust-to-gas ratios reported in Table 2) and scaled the masses \textit{ex post facto} to achieve the targeted aggregate state. This mass scaling factor can be interpreted as the fraction of dust in the dynamical state compared to the aggregate state, such that the combined (dynamical + aggregate) dust-to-gas ratio

\(^5\) Although infalling grains consist of a mixture of all grain types, adding small ISM grains to the silicate grain-size distribution has a negligible effect on the mass distribution of silicates in the disc, which is dominated by the large aggregates. On the other hand, even a small increase in the dynamical mass of presolar grains can have a significant impact on local isotopic ratios.
Equations (4) and (6): little the presolar grains contribute to the composite mass. Furthermore, to the intrinsic density, but these changes can be safely ignored given how small the presolar grains contribute to the total solid content in the disc and 

\[
\frac{\Delta \rho}{\rho} = \frac{1}{\epsilon} \sum_j \epsilon_j \Delta v_j,
\]

where \(\Delta \rho\) and \(\rho\) are the mass fractions (relative to the mixture) of the individual and combined dust phases, respectively.

\[\epsilon_j \equiv \frac{\rho_{d,j}}{\rho},\]

\[\epsilon \equiv \sum_j \epsilon_j = \frac{\rho_d}{\rho},\]

\[\Delta v_j \equiv v_{d,j} - v_g.\]

The result by the abundance ratios \(\chi_{\text{Si}}\) and \(\chi_{\text{Ox}}\) as follows:

\[\frac{\Delta \rho}{\rho} = \frac{1}{\epsilon} \sum_j \epsilon_j \Delta v_j,\]

\[\Delta v_j = \left( \frac{\Delta f_j}{\rho} \right) \frac{1}{\epsilon - \epsilon_j},\]

where \(\Delta f_j\) is the differential velocity 

\[\frac{\Delta \rho}{\rho} = \frac{1}{\epsilon} \sum_j \epsilon_j \Delta v_j,\]

\[\Delta v_j = \left( \frac{\Delta f_j}{\rho} \right) \frac{1}{\epsilon - \epsilon_j},\]

\[\epsilon_j \equiv \frac{\rho_{d,j}}{\rho},\]

\[\epsilon \equiv \sum_j \epsilon_j = \frac{\rho_d}{\rho},\]

\[\Delta v_j \equiv v_{d,j} - v_g.\]

\[f\] represents accelerations acting on both components of the fluid while \(f_{d,j}\) and \(f_{d,j}\) represent the accelerations acting on the gas and dust components, respectively, \(\Delta f_j \equiv f_{d,j} - f_{g,j}\) is the differential force between the gas and each dust phase, \(v_{d,j}\) is the stopping time specific to each grain type (see Equation 18), \(u\) is the specific thermal energy of the gas, and \(P\) is the gas pressure. Importantly, the backreaction from each dust phase onto the gas is inherently accounted for in Equation (11), including the subsequent feedback of the cumulative result in the gas back onto each dust phase. Thus, while there is no direct coupling between dust phases, they do interact via their common coupling to the gas.

2.3.2 Gas

We employed a vertically-isothermal disc with radial power-law profiles for the total (gas + dust) surface density, \(\Sigma = 2 \zeta_0 (R/R_0)^{-P}\), and the sound speed, \(c_s = c_{s,0} (R/R_0)^{-\eta}\). The gas surface density is related by \(\Sigma_g = (1 - \epsilon) \Sigma\). Here we have used the subscript 0 to denote the reference value taken at a cylindrical distance \(R_0\) from the central star of mass \(M = M_\odot\). Defining the disc scale height as \(H = c_s/\sqrt{G\Sigma}\), where \(\sqrt{G\Sigma}\) is the gravitational constant, the aspect ratio for our disc is \(h = H/R = h_0 (R/R_0)^{-\eta}\). The gas equation of state is given by \(P = \frac{\gamma}{\gamma - 1}\frac{\rho}{\rho}c_s^2\). Lastly, the gas viscosity in PHANTOM is governed by the artificial dissipation parameters \(\alpha_{AV}\) and \(\beta_{AV}\) (Price et al. 2018).

Note: The text contains mathematical equations and references which are not fully rendered in the text format provided. The equations are part of the scientific discussion and are essential for understanding the context and methodology used in the research. The references cited at the end of the text are crucial for further reading and verification of the methodologies and results presented.
The latter is fixed at $\beta_{\text{AV}} = 2$ to prevent interpenetration of particles while the former can be indirectly related to the Shakura-Sunyaev viscosity $\nu = \alpha_{\text{SS}} c_s H$ via the relation (Lodato & Price 2010):

$$a_{\text{SS}} \approx \frac{a_{\text{AV}} (\text{bkg})}{H}$$

where $(\text{bkg})$ is the mean smoothing length of particles in a cylindrical ring at a given radius.

As our fiducial setup we chose a disc with a radial range $R \in [0.3, 100] \text{ au}$ and a reference radius $R_0 = 1 \text{ au}$. We set the total disc mass to $M_{\text{disc}} = 0.05M_\odot$, the power-law indices for the disc to $p = 1$ and $q = 0.25$, and the reference aspect ratio to $h_0 = 0.05$. The resulting reference surface density and sound speed were $\Sigma_0 = 792 \text{ g cm}^{-2}$ and $c_{s,0} \approx 1.5 \text{ km s}^{-1}$, respectively. Using $2 \times 10^6 \text{ SPH particles}$ and $a_{\text{AV}} \approx 0.07$, we obtained a radial average Shakura-Sunyaev viscosity parameter $(\alpha_{\text{SS}}) \approx 1 \times 10^{-3}$ (the complete range in the disc spanning $[0.5, 9] \times 10^{-3}$).

2.3.3 Dust

The terminal velocity approximation inherently assumes that dust is well coupled to the gas or, more quantitatively, that the Stokes number of each grain size $St_j \equiv \tau_j \Omega_k \ll 1$. In this regime, the stopping time $\tau_j$ is aptly modelled using Epstein drag (Epstein 1924):

$$\tau_j \equiv \frac{\rho_{\text{grain}} \gamma_j}{\rho_{\text{gas}}} \sqrt{\frac{\pi \gamma}{8}},$$

which is suitable for spherical dust grains smaller than the mean free path of the gas and that travel at subsonic velocities with respect to the gas.7

When $St_j \gtrsim 1$, the terminal velocity approximation breaks down (with errors on the order of $\gtrsim 10\%$; see Laibe & Price 2014a) and the timestep stability criterion compensates by becoming prohibitively small (Price & Laibe 2015; Hutchison et al. 2018; Ballabio et al. 2018). The low-density upper and outer disc regions are particularly susceptible to these numerical issues. More problematically, instabilities can occur if large dust grains get flung out and trapped in these regions. We followed Ballabio et al. (2018) in circumventing these issues by setting a maximum threshold on the stopping time of weakly-coupled grains.

In order to model the three dust populations simultaneously, we had to modify PHANTOM to allow different intrinsic densities. Because each grain size only directly interacts with itself and the gas, we only needed to expand the constant $\rho_{\text{grain}}$ into an array. Another minor change we made to the code was in the parameterisation of the dust-to-gas ratio (see Appendix A for more details). We benchmarked and tested all of the changes we made to the code using the test suite described in Price et al. (2018).

The initial dust properties (e.g. size, density, and dust-to-gas ratio) for the 17 dust species were discussed previously in Section 2.2. In our fiducial setup, we assumed a global dust-to-gas ratio of $e = 0.01$ for the disc and uniformly initialised each simulation particle with the dust-to-gas ratios in Table 2. This implies that all dust grains, presolar and silicates alike, are uniformly distributed in the disc. While there is some evidence for spatial and/or temporal variations in the inheritance of presolar grains during infall (e.g. Nanne et al. 2019; Haba et al. 2021), assuming a uniform initial distribution simplified the analysis and allowed us to focus on the dynamics rather than the (largely unconstrained) initial distribution. We found further support for these initial conditions when looking at the mixing of small dust grains (Section 3.2.2), especially if the early disc was massive enough for gravitoturbulence to operate (see Section 4.2.1). One initial condition that we did vary was the total dust-to-gas ratio. In an effort to enhance the effects of backreaction we ran a few simulations with $10\times$ more dust (i.e. $e = 0.1$), in which case the dust-to-gas ratios in Table 2 should be multiplied by 10.

In many studies, it is customary to relax the gas disc before adding the dust in order to avoid potential influences from the slight non-equilibrium in the initial conditions. However, the presolar grains are so small, they are able to relax together with the gas without being affected by initial perturbations. This is not necessarily true for the larger silicate grains, but for purposes of this study we are only interested in the relative differences that develop between dust types (presolar versus silicates) or between simulations (single- versus multi-grain). Therefore, as long as the initial conditions are consistent, we can forego relaxation and initialise all of our simulations with dust from time $t = 0$.

2.3.4 Backreaction with multiple grain sizes

The dynamics of each dust phase can be modelled as a collisionless fluid suspended in a gas that evolves independently of other grain sizes. Even when coagulation and fragmentation are considered, the dynamics of each dust phase as an ensemble remains approximately\(^8\) intact. Drag between the gas and dust leads to an exchange of angular momentum (drag heating is negligible), the magnitude of which depends on the local mass density and differential velocity of the dust with respect to the gas. The effects of drag are more visible in the dust phases because the gas dominates the mass budget in the disc, but there is an equal and opposite reaction in the gas that is referred to as backreaction. Going one step further, the accumulated backreaction from multiple dust grains exchanging momentum with the same gas phase creates a feedback loop that indirectly couples the dynamics of dust grains of different sizes. For example, large grains may experience a headwind from the gas that causes them to lose angular momentum and migrate inward while the backreaction pushes the gas radially outwards. As the gas moves outward, it drags small, tightly coupled dust grains in its wake, thereby indirectly coupling the dynamics of small and large grains together.

In like manner, dust can be indirectly linked to any other disc process that affects the gas, such as viscous evolution. Several studies have analytically explored the effect of backreaction and viscosity on the dust dynamics in discs, but usually under restrictive assumptions. For example, linear stability analysis has demonstrated the importance of viscosity and backreaction in the operation of the streaming instability inside pressure maxima (Jacquet et al. 2011; Auffinger & Laibe 2018), but only on local scales. On global scales, analytic solutions have been obtained for the migration rates of (i) independent dust grains in a viscous disc (i.e. no backreaction; Takeuchi & Lin 2002), (ii) coupled dust grains in an inviscid disc (Bai & Stone 2010) and, more generally, (iii) coupled grains in a viscous disc (Dipierro et al. 2018). However, even in this most general case, Dipierro et al. could only find agreement with numerical simulations in which the power-law disc structure was preserved,\(^8\)

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7 Although not important for this study, the drag prescription in PHANTOM accounts for the correction factor for supersonic drag (Kwok 1975) and the transition to Stokes drag (e.g. Whipple 1972; Weidenschilling 1977).

8 The mass transfer between grains of different size can have long term effects on the dynamics in the disc.
something they achieved in their simulation by artificially halting dust migration.

Numerous numerical studies have investigated backreaction in viscous discs under less idealised conditions. Viscosity and backreaction has been a common ingredient in numerical simulations of protoplanetary discs for decades (e.g. Shakura & Sunyaev 1973; Weidenschilling 1980). In the intervening years, backreaction has proven to be a key factor in the streaming instability (Youdin & Goodman 2005; Youdin & Johansen 2007), vortices (Fu et al. 2014; Crnkovic-Rubasmens et al. 2015; Surville et al. 2016), and pressure maxima (Taki et al. 2016), the last of which can be produced by planet gaps (Weber et al. 2018), disc instabilities (e.g. the magnetorotational instability; see Kretke et al. 2009; Kato et al. 2012), snow lines (Okuzumi et al. 2012), and self-induced dust traps (Gonzalez et al. 2017; Pignatale et al. 2017). Backreaction from multiple grain sizes has been achieved in some of these studies by tracking the size evolution of dust grains as they grow/fragment in the disc. While this is a good way of tracking the evolution of individual grains, it makes it difficult to disentangle the effects of backreaction on a given grain size or range of grain sizes (e.g. presolar grains), and thus not very useful to our current study.

To clarify how backreaction affects grains of different sizes in our simulations, we kept our grain sizes fixed and used a pre-grown silicate grain population (as described in Section 2.2) to provide the bulk of the backreaction for our disc. In so doing, we inherently assumed that our grain-size distributions were in a steady state. Realistically one would expect dust to grow rapidly on timescales of 100s–1000s of years (e.g. Birnstiel et al. 2016) and, although this is a good way of tracking the evolution of individual grains, it makes it difficult to disentangle the effects of backreaction on a given grain size or range of grain sizes (e.g. presolar grains), and thus not very useful to our current study.

2.3.5 Sink particles

We modelled the central star and planet using sink particles (Bate et al. 1995). The accretion radius for the star was set to the inner radius of the initial disc. When present, a Jupiter-mass planet was embedded in the disc at \( R_p = 10, 20, \) or 40 au (none of which are meant as a model for Jupiter in the solar system). The accretion radius of the planet was set to 1/4 of the planet’s local Hill sphere. In each simulation, the planet was free to migrate according to planet-disc interactions and viscous disc evolution. We did not relax the system when embedding the planet in order to ensure we started with the same initial conditions as when the planet was absent (to facilitate comparison of the dust evolution between the different simulations).

2.4 Calculation of isotopic compositions

2.4.1 Choice of isotopic systems

To capture the potential nucleosynthetic variations created by tracking the presolar grain dynamics relative to the background silicate population, we gavethe silicates a terrestrial\(^9\) isotopic composition and ‘painted’ our presolar grains with two of the following three isotopic elements: \(^{54}\)Cr, \(^{96}\)Zr, and \(^{50}\)Ti.

The isotope \(^{54}\)Cr is likely produced by massive stars that exploded as Type II SNe (e.g. Dauphas et al. 2010; Qin et al. 2011). This isotope is proposed to be enriched in oxide grains, mainly presolar spinels (Dauphas et al. 2010; Qin et al. 2011; Nittler et al. 2018; Zinner et al. 2003); thus, we assume \(^{54}\)Cr is carried by the oxide grains in our simulations. The input data for \(^{54}\)Cr/\(^{52}\)Cr ratios of presolar oxides grains from Hynes & Gyngard (2009), and reference therein, supplemented by individual publications (Nittler et al. 2018; Dauphas et al. 2010; Qin et al. 2011). The grains presented in Nittler et al. (2018) are rare but have extremely high \(^{54}\)Cr/\(^{52}\)Cr ratios, We assumed that they constitute up to 30% of presolar oxides. This is considered to be an upper limit.

\( Zr \) is the most abundant heavy element in mainstream SiC grains (Amari et al. 1995). The \( Zr \) isotopes \(^{90}\)Zr, \(^{91}\)Zr, \(^{92}\)Zr, and \(^{94}\)Zr are dominantly synthesized by the \( s \)-process (e.g. Nicollusi et al. 1997; Schönbächler et al. 2003), while the production of \(^{96}\)Zr requires higher neutron fluxes, which can occur in diverse stellar settings (e.g. Akram et al. 2015). Although the \( s \)-process may have contributed up to 82% of the production of \(^{96}\)Zr (Bisterzo et al. 2011; Travaglio et al. 2004), other processes are needed to produce the remaining \(^{96}\)Zr found in the solar system such as the weak \( r \)-process or charged-particle reactions (CPR, e.g. Kratz et al. 2008; Akram et al. 2013). It has been shown that distribution of \(^{96}\)Zr variations in solar system materials reflects the heterogeneous distribution of \( s \)-process material (Akram et al. 2015; Ek et al. 2020). The \(^{96}\)Zr/\(^{94}\)Zr ratio for the SiC grain population was determined using the weighted averages of the compositions of the different types of SiC grains for which data is available, predominately mainstream and some minor (1 %, Zinner 2014) X SiC grains (Hynes & Gyngard 2009).

The isotope \(^{50}\)Ti is produced in various settings, such as rare Type Ia SNe, core-collapse Type II SNe, and AGB stars (Clayton 2003). We therefore assume it is carried by both SiC and oxide grain populations. In mass balance calculations for \(^{50}\)Ti, we used isotopic data collected in Hynes & Gyngard (2009) for SiC and oxide grains.

2.4.2 Mass balance equation

The nucleosynthetic variations recorded in meteorites reflect the isotopic ratios that were present in the various regions of the disc in which they were formed (likely controlled by the concentration of presolar grains relative to the solar system silicates; e.g. Ek et al. 2020). Having assigned different isotopic compositions to each dust type, it is straightforward to calculate the isotopic ratios resulting from the final surface densities of oxide, SiC, and silicate grains in our simulation. To this end, we used the following mass balance equation:

\[
\left( \frac{X}{\Xi} \right)_{\text{tot}} = \sum_i n_i \left( \frac{X}{\Xi} \right)_i,
\]

Where \( n_i \) is the number density of the isotope \( X \) in the \( i \)-th component and \( \Xi \) is the total mass density. The subscript \( \text{tot} \) indicates that the mass balance is calculated for the total mass of the disc.

\(^9\) We make the assumption that terrestrial compositions are equivalent to the average solar composition and hence ISM compositions, although this is not strictly correct. We do not know the isotopic composition of the ISM or solar compositions at the level of precision we can measure in meteorites. However, for purposes of calculating the isolate mixture, this is not important because the presolar grains are so different in their isotopes. A slightly different ISM (or solar) composition will not affect the isotopic abundances we are interested in because the presolar grains dominate the results.
where $y$ and $z$ are the mass numbers of two isotopes of element $X$ and $f_i$ is the fraction of the most abundant isotope of element $X$ carried by dust species $i$ (i.e. oxide, SiC, or silicate grains). This fraction is calculated as follows:

$$f_i = \frac{M_i C_i^X}{\sum_j M_j C_j^X}.$$  

(20)

where $M_i$ is the molar mass of element $X$ and $C_j^X$ is the concentration of the most abundant isotope of this element in the system. Because $M_i$ conveniently appears in both the numerator and denominator, the area factors needed to convert the molar mass into surface density cancel and we can replace $M_i$ directly with the corresponding surface density $\Sigma_i$ from the simulation. All values used for these equations are summarised in Appendix B.

3 RESULTS

Using the setup for the gas and dust described in the previous section, we performed a series of multi-grain simulations to compare the dynamics of our three dust populations when (i) the dust-to-gas ratio is $\varepsilon = 0.01$ and no planet is present in the disc (fiducial simulation), (ii) the dust-to-gas ratio is arbitrarily increased by a factor of 10, and (iii) a Jupiter-mass planet is introduced at various locations in the disc. Since drag and viscosity are the two main drivers of evolution in our simulations, we first isolate their individual contributions, then we show how their combined effects produce isotopic variations during the course of ordinary disc evolution.

3.1 Drag effects

To isolate the effects of drag from viscosity (particularly backreaction), we performed additional single-grain simulations for grains $j = \{3, 7, 8, 13, 16, 17\}$ (see Table 2) for every multi-grain simulation we ran. We selected these sizes to cover a broad range in Stokes numbers and to have at least one representative grain size from each population. By keeping the gas and the selected dust density the same as in the multi-grain simulation we can attribute the differences between the single- and multi-grain simulations to the cumulative backreaction from having multiple dust sizes or, in other words, the indirect feedback between grains of different sizes. Figure 2 compares surface density profiles from single- and multi-grain simulations for three different setups (from top to bottom): no planet, a Jupiter-mass planet initialised at $a = 10$ au, or alternatively initialised at $a = 40$ au. For clarity, only a subset of silicate grains are shown. The presolar grains all have radial profiles that are almost identical to the $s_8$ case,\(^\text{10}\) but offset vertically according to the dust-to-gas ratios in Table 2. The strong variability in the inner disc is a numerical effect caused by having too few particles in this region (a boundary effect from having a large accretion radius for the central sink particle). In the bulk of the disc, the most visible differences between the single- and multi-grain simulations are unsurprisingly localised to regions where the dust-to-gas ratio

\(^\text{10}\) Normalising and overlaying the curves for $j = \{3, 7, 8\}$ reveals small differences within the planet gap and in the outer disc ($R > 100$ au), primarily due to the difference in grain size. More importantly, however, the relative difference between single- and multi-grain simulations for all three cases is indistinguishable and the $s_8$ case is sufficient to illustrate the effects of backreaction on all of the smaller grains in the disc.

Figure 2. Radial surface density profiles for silicate grains $j = \{8, 13, 15, 16, 17\}$ after 17 000 yr of evolution in a disc with either no planets (top) or a Jupiter-mass planet initialised at 10 au (middle) or 40 au (bottom). Each panel contains a multi-grain simulation with a dust-to-gas ratio of $\varepsilon = 0.01$ (solid lines) and matching single-grain simulations (dashed lines). The top panel additionally shows a multi-grain simulation with $\varepsilon = 0.1$ (dotted lines), rescaled to the fiducial dust-to-gas ratio for better comparison. The small differences between the multi-grain and single-grain simulations suggests that cumulative backreaction does not significantly affect the dust surface density in the disc until the largest grains form a local concentration of $\varepsilon \gtrsim 0.1$. Meanwhile, viscous expansion efficiently pulls smaller grains into the outer disc where they can potentially grow and drift in again. For reference, the vertical grey line gives the outer edge of the initial disc.
is high ($\varepsilon \gtrsim 0.1$), typically near the density maxima for the largest grain size because it dominates the solid mass distribution.

Globally speaking, the indirect coupling between dust grains via their mutual backreaction onto the gas tends to have one of two effects. Either the grains are dragged outwards by the gas or they experience a slower migration rate from the reduced relative velocity between the gas and the dust. In the former case, the outward migration produces a deficit in the surface density of the dust (see $s_{16}$ and $s_{15}$ grains), the width and the depth of the depletion being related to the width and enhancement of the dust-to-gas ratio. In the latter case, the peak dust densities are shifted slightly to larger radii (compare the density maxima for the $s_{16}$ grains) or, when combined with the shepherding influence of a migrating planet, the retarded migration rate allows more dust to be swept up and trapped in the moving pressure bump on the inner rim of the gap (see the $s_{15}$ grains in the bottom panel; also observed in the $s_{14}$ grains, not pictured).

3.1.1 Increasing the dust-to-gas ratio

The above results indicate that the local dust-to-gas ratio has a strong influence on the strength of the backreaction in the disc. We tested this further by increasing the dust-to-gas ratio of each grain by a factor of 10, for a total of $\varepsilon = 0.1$. The results from this simulation are displayed as dotted lines in the top panel of Figure 2, but have been scaled down by a factor of 10 to better compare with the fiducial setup. Note that because we raised the dust-to-gas ratio without changing the overall disc mass, some of the global differences with the fiducial model can be partially attributed to having a smaller gas mass in the disc; however, the large differences seen in the inner disc can only have been caused by backreaction.

Large grains tend to have the largest dust-to-gas ratios and, hence, provide the bulk of the backreaction onto the gas. On a subtler level, their coupling with the gas is balanced in a way that delivers maximum effect to the gas: it is neither so strong as to force equilibration nor so weak as to prevent momentum exchange. Incidentally, these same properties (i.e. large inertia and weak drag) also make the larger grains less susceptible to the dynamical feedback from the gas (whether self induced or from other grain sizes). This explains why we did not observe any changes in the $s_{17}$ grains until we raised the dust-to-gas ratio. Unlike the fiducial disc where we had to wait $\gtrsim 10^4$ yr before any $s_1$ reached a threshold (~few percent) where the effects of backreaction could be visible, the largest grains in the $\varepsilon = 0.1$ case started near this threshold and backreaction could take effect as soon as dust began to accumulate. The prolonged and heightened outward migration of gas from the inner disc not only depleted the small grains more severely than before, but also triggered faster migration of the larger grains in this region. As a result, the initial peak density of $s_{17}$ grains in the inner disc was, when scaled, both larger and closer to the central star than in the fiducial case. Over time this proximity to the inner boundary led to a significant loss of dust and a deficiency in $s_{17}$ grains in the inner disc.

It is interesting to note that, even after increasing the dust-to-gas ratio, the backreaction from the $s_{17}$ grains clearly dominated over the contributions from other grain sizes. Undoubtedly, if left to evolve longer, the further concentration of $s_{16}$ grains would play a bigger role. Alternatively, if the $s_{17}$ grains had been removed, the $s_{16}$ grains would have taken over as the dominant grain size controlling the backreaction onto the gas, albeit with less efficiency. This hierarchy of the largest grain size controlling the backreaction is established by (i) the decreasing susceptibility to and increasing influence on backreaction as grain size increases and (ii) the local grain size distribution. The first is an immutable property of aerodynamic drag, but the second is strongly influenced by our dust model (e.g. the choice of $P$, radial drift, grain growth and fragmentation), thus highlighting the importance of self-consistently setting the local maximum grain size in the disc. Furthermore, since backreaction is a cumulative effect, the initial conditions (e.g. the grain size distribution, the dust-to-gas ratio, the presence of a planet) can impact when, where, and how strongly backreaction affects the gas and dust evolution.

3.2 Viscous effects

Viscosity influences the dust by driving the gas evolution in the disc in the form of radial migration, diffusive mixing, and viscous expansion.

3.2.1 Radial migration

Snapshots of the radial velocities for the gas and presolar grains are shown in Figure 3 for the case of a Jupiter-mass planet initialised at 10 au. When viewed face on, the radial velocity pattern traces the spiral density waves created by the planet (left panel), which are well known for transporting angular momentum in the disc. The resulting sinusoidal oscillation in the flow direction shows up as alternating vertical bands in the azimuthally-averaged vertical cross-section (middle panel; see also e.g. Bae et al. 2016), but have limited influence on the average radial velocity of the presolar dust grains near the disc mid-plane (far right panel). This influence is slightly more pronounced when initialising the planet at 40 au (grey dashed line) because the banded vertical structure is better defined and covers a larger region of the disc. In this latter case, the peaks and troughs in the velocity profile outside of $R > 25$ au correlate with the locations of the positive and negative vertical bands, respectively, although the mean remains consistent with the smooth, monotonically increasing no-planet case (grey dotted line). In stark contrast, the three cases show little agreement in the radial velocities interior to the planet location. Embedding the planet at 10 au produces inward migration in the inner disc while inserting the planet at 40 au enhances the outward migration (due to the feedback from backreaction of larger grains that have accumulated in the inner disc; see bottom panel in Figure 2). In all of this, the only place size/density sorting of presolar grains (or other small silicate phases) takes place is outside the main disc where the gas densities drop exponentially and the Stokes numbers exceed $St \gtrsim 0.01$.

3.2.2 Diffusive mixing

In addition to the bulk radial motions of the gas and dust, viscosity is also an efficient source of diffusive mixing within the disc. Diffusion works to homogenise local gas and dust concentrations (chemical or otherwise), slowly erasing the dynamical history that created them. This is perhaps best demonstrated by tracing the positions of a localised group of particles as they evolve in time. Figure 4 shows one such configuration that we traced, consisting of presolar grains located within a torus with a major radius of 20 au (centred on the star) and a minor radius of 1 au (centred at $z = 0$). This grouping was chosen because of its proximity to the planet location at the end of the simulation in order to highlight the exchange of material across the planetary gap (in some cases as many as nine times). In this somewhat extreme example, the initial concentration was strewed across $R \lesssim 50$ au in only a few thousand years – primarily due to
interactions with the planet but also through diffusive spreading and subsequent rapid transport via surface flows.

We quantified the diffusive spreading using the root-mean-square displacement of both inner and outer reservoirs, which under 2D Fickian diffusion is proportional to the square root of the time: \( r_{\text{rms}} = \sqrt{4Dt} \). By fitting \( r_{\text{rms}} \), we inverted the equation to find diffusion coefficients of \( D \sim 3\times10^{-4} \) au\(^2\) yr\(^{-1}\) for the inner and outer reservoirs, respectively. Despite the interfering influence of the planet, these values are roughly consistent with the expected gas diffusion assuming a Schmidt number \( Sc \sim 1 \) (e.g. Johansen et al. 2006; Desch et al. 2017): \( D \sim \nu/Sc \sim \rho_S \Omega_k H/\rho \). Note that here \( \alpha_S \) is the local disc value and not the disc averaged value of \( 10^{-3} \) (see Section 2.3.2). In locations farther from the planet, or in the case where the planet was absent, we found agreement to within \( \lesssim 10\% \). Thus the timescale for vertical diffusion \( (\tau_{\text{diff}} \sim H^2/D) \) in our model varies from \( \sim 100 \) yr in the inner disc to \( \sim 10^3 \) yr in the outer disc. Note this is comparable to estimates of the growth timescale for dust: \( \tau_{\text{grow}} = C'(\Omega_k r_0)^{-1} \), where \( C' \) is a model parameter of order \( \sim 10 \) (Brauer et al. 2008a).

Finally, once the small grains had been diffusively mixed into the upper disc layers, surface flows rapidly transported these grains radially inward. This transition can be observed for the inner reservoir at \( t = 3000 \) yr, where two finger-like protrusions extend radially inward along the surface of the disc. As time evolves, these dust grains were either accreted by the central star or diffused back into the disc. Homogenisation of the inner disc was further accelerated...
by the migrating planet, which pushed material radially inwards and increased the supply of dust to the surface flows. We observed qualitatively similar behaviour in the outer reservoir, but now with the planet taking the role of the central star by accreting incoming material (as opposed to driving the flow from the outer boundary) and impeding surface flows from delivering dust grains across the gap. This can be seen by the accelerated decline in the number of fluid parcels in the outer reservoir after $t > 8000$ yr despite the growing separation between the planet (migrating inward) and the dust centroid (migrating outward). However, unlike the inner disc, full homogenisation of the region between the planet and the centroid did not occur due to (i) the surface flow being limited by diffusive mixing (i.e. there was no exterior planet to help with feeding) and (ii) the diffusive timescale increasing with radius. Nevertheless, these results show that diffusion and radial transport via surface flows can be an effective means for redistributing small dust grains in the disc.

3.2.3 Viscous expansion

Strictly speaking the outward expansion of gas and dust is a combined effect of viscosity and backreaction, but the near perfect agreement between simulations at radii $R > 100$ au in Figure 2 suggests that backreaction plays a minor role in disc expansion and the transport of small dust grains in the outer disc. This was demonstrated analytically by Dipierro et al. (2018), but here the evolution also played a role by removing the large grains from the outer disc, thereby diminishing the effect of backreaction even more. Another contributing factor to expansion in our simulations was the initial pressure discontinuity at the outer edge of the disc ($R = 100$ au), but these effects were short lived (few 1000 yr) and viscous spreading soon took over as the dominant expansion mechanism.

Figure 5 shows the temporal evolution of the surface density of the gas and three representative dust grains ($j = [3, 12, 17]$) at 1000 yr intervals. The majority of dust mass pulled out in the initial wake quickly stalled in the low-density environment outside the disc and simply resumed its usual inward migratory behaviour (Panel D). However, while the dust fronts of the larger grains moved radially inward, those of the smaller grains moved steadily outwards (Panel B) as viscous expansion siphoned away tightly-coupled dust grains with the gas. Intermediate-sized grains (Panel C) decoupled from the gas soon after being pulled from the disc and piled up between $R = 100 – 140$ au.

3.3 Isotopic ratios

We obtained radial profiles for our three isotopic ratios by inserting the surface densities from our multi-grain simulations into Equations (19) and (20). Because the magnitude of the resulting ratios are so small, we give them in $\epsilon$ notation \footnote{Not to be confused with the $\epsilon$ used for the dust-to-gas ratio. Confusion can be avoided by noting that the $\epsilon$ in isotopic ratios is always written together with the corresponding isotope.}, $\epsilon X$, which corresponds to 1 per 10 000 with respect to some standard (as opposed to the often used $\delta$ notation given in $%\epsilon$). This allows a direct comparison with the literature data from meteorites. The conversion to $\epsilon$ notation is calculated according to

$$
\epsilon X = \frac{\left(\frac{X}{X}\right)_{\text{sample}} - 1}{\left(\frac{X}{X}\right)_{\text{standard}}} \times 10 000,
$$

(21)

Figure 5. Time series of the radial surface densities for the gas (Panel A) and dust grains ($j = [3, 12, 17]$) (Panels B–D) in the outer disc at 1000 yr intervals. The initial expansion and relaxation of the surface density in the bulk disc was rapid ($< 2000$ yr), although it took another ~4000 yr for the radial dust velocities in the disc to fully settle. Small grains ($j = 1–11$) were dragged out of the disc by viscous expansion of the gas, leading to a steady increase in surface density beyond $R > 100$ au (Panel B). Intermediate grains ($j = 12$) piled up outside the main disc at $R \leq 140$ au (Panel C). Large grains ($j = 13–17$), initially pulled out during the initial expansion of the disc, stalled in the low density environment and resumed their usual inward radial migration (Panel D).
where \( \epsilon \)\text{sample} and \( \epsilon \)\text{standard} distinguish between measurements in the sample and the normalising standard of terrestrial origin. While earlier we could get away with using approximate ISM compositions in the mixing calculations (see Footnote 9 on Page 7), by switching to epsilon notation we move into a high precision regime where small relative differences matter. Hence, for each simulation, we recalculate the isotopic differences relative to Earth at 1 au, as is typically done for meteorite data.

The isotopic ratios calculated in the disc are very sensitive to the dynamical mass in the presolar grain populations. Using the formalism we developed in Section 2.2.3, we explored two opposite extremes with regard to the inclusion of presolar grains into larger aggregates in the disc. In the most liberal case, we assumed the dynamical mass contains 100% of the presolar grains in the disc. In the more conservative extreme, we set \( \epsilon_{\text{coag}} = 10 \mu m \) such that all silicates greater than 10 \( \mu m \) contained a fixed abundance ratio of presolar grains. From Equation (4), this is equivalent to having ~97.14% of presolar grains in the aggregate mass. We will refer to these two scenarios by the mass reservoir that contains the most presolar mass: the dynamical and aggregate cases, respectively.

The isotopic compositions we computed for \( \epsilon^{54}\text{Cr} \), \( \epsilon^{50}\text{Ti} \), and \( \epsilon^{96}\text{Zr} \) are shown in different columns of Figure 6, with the dynamical and aggregate cases appearing in the top and bottom rows, respectively. As mentioned above, each curve in the aggregate case is normalised to Earth at 1 au in order to be consistent with meteorite measurements; however, because the variations in the dynamical case are much larger than most of the solar system measurements, we normalised these curves to ISM compositions because the similarities and differences between simulations are then easier to observe. Despite these differences in normalisation, we can finally see the effect mentioned earlier that shifting mass between the dynamical and aggregate mass reservoirs only affects the magnitude of the isotopic variations, not the radial profile. Retaining all of the presolar grains in the dynamical state produced variations that rapidly surpassed solar system measurements, indicating that at least some form of aggregation is needed to explain solar system abundances. The magnitude of peaks in the aggregate case were reduced on average by a factor of ~33 relative to the dynamical case, putting them more in line with solar system measurements. Because of the lack of size/density sorting between presolar grains, the radial profiles

Figure 6. Radial profiles resulting from mass balance calculations for \( \epsilon^{54}\text{Cr} \) (leftmost column), \( \epsilon^{50}\text{Ti} \) (middle column), and \( \epsilon^{96}\text{Zr} \) (rightmost column) at \( t = 17 \, 000 \) yr. Grey lines correspond to simulations with different initial planet locations. As in previous figures, the final position of the planet is marked with an image of Jupiter. Top row: values calculated for the dynamical case, where all presolar grains (oxide and SiC) are kept separate from the silicates. Isotopic ratios are normalised to ISM compositions to emphasise the similarities and differences between simulations, namely the variation in the inner disc, the peaks associated with the planet, and the universal agreement in the outer disc. Bottom row: values from the aggregate case, where ~97% of presolar grains are trapped within silicate aggregates. Symbols corresponding to measured compositions in the solar system are given for comparison, including: Earth; the Moon; enstatite chondrites (EC); Mars; ordinary chondrites (OC); howardites, eucrites, and diogenites (HED); and carbonaceous chondrites (CC). Isotopic ratios are normalised to Earth at 1 au to be consistent with meteorite measurements that do the same. Meteorite measurements are also included in the top row despite the inconsistent normalisation (emphasised by using semi-transparent symbols) in order to accentuate the difference in scales between the dynamical and aggregate cases. Available data for solar system objects have been collected from Trinquier et al. (2007) in the case of \( \epsilon^{54}\text{Cr} \); Zhang et al. (2011, 2012), Gerber et al. (2017), and Trinquier et al. (2009) in the case of \( \epsilon^{50}\text{Ti} \); and Akram et al. (2015) in the case of \( \epsilon^{96}\text{Zr} \). Additionally, data for platy hibonite crystals (PLACs; Kööp et al. 2016) are given in the middle panel to show that some materials require much larger variations than even our most extreme case (maximum and minimum values are indicated by blue arrows next to the data points). Such crystals are predicted to form very close to the Sun, but because of the logarithmic scale, we placed them at 1 au. Assumptions for the location of EC, OC, and CC meteorites are described in Section 4.3.
for each isotope were similar to one another (although mirrored across the origin in the case of $\varepsilon^{50}$Ti), with variations occurring in the inner and outer disc in every one of our simulations. The only major deviation from this symmetry between isotopes was outside of the main disc at $R \sim 170$ au where the decreasing trend in $\varepsilon^{96}$Zr suddenly reverses direction, whereas $\varepsilon^{54}$Cr and $\varepsilon^{50}$Ti continue to increase monotonically until $R \sim 230$ au.

The radial extent and magnitude of the variations in the inner disc showed a mild sensitivity to the planet’s location. Further out, the gap in large grains carved by the planet created an additional peak in the isotopic ratios that migrated together with the planet through the disc. The intensity and width of this peak varied with the initial planet location, as detailed in Table 3. On either side of this peak, the isotopic ratios were pinned to ISM values by the concentration of silicate grains in the inner and outer pressure bumps that act as dust traps for larger grains. Note that unless there is a mechanism to locally enrich large aggregates in presolar grains, the dust traps created by a massive planet (e.g. Jupiter) will not be able to produce isotopic variations due to the dilution from silicates that concentrate there. Such enrichment may be possible from the steep increase in isotopic variations we observed in the outer disc. These variations were unperturbed by the presence and location of the planet and thus very robust – especially considering their natural origin from generic evolutionary processes within the disc (i.e. viscosity and drag).

4 DISCUSSION

4.1 Origin of isotopic variations

In Sections 2.1 and 2.2 we spent a lot of effort accounting for differences in grain size distribution and mean density for the oxide, SiC, and silicate dust populations for the intent of tracking relative changes between dust phases that might lead to isotopic variations in the disc. Although these differences in intrinsic dust properties resulted in size/density distribution and mean density for the oxide, SiC, and silicate dust populations for the intent of tracking relative changes between dust phases that might lead to isotopic variations in the disc. However, as such, they provide a robust mechanism by which variations can build up and/or be reinforced over the lifetime of the disc, even when starting from a homogeneously distributed background of presolar grains.

The source of the isotopic variations in our simulations comes from a combined effect of drag and viscosity. We use the general term ‘drag’ because all aspects of drag can play a role (in order of decreasing significance): radial drift, vertical settling, and backreaction, the last of which indirectly couples the dynamics of different dust phases by being immersed in the same gas phase. Radial drift transports large quantities of silicates into the inner disc in the form of large aggregates that have vertically settled to the mid-plane. As the dust-to-gas ratio at the mid-plane increases, gas is pushed radially outwards through backreaction, dragging with it presolar grains and other small silicates. Crucially, it is the isotopic ratio within these small grains and their motion relative to the bulk silicates that drives the isotopic heterogeneity in the disc. At the most basic level, the concentration of silicates relative to a uniform background of smaller grains can dilute isotopic signatures in the inner disc and enhance them in the outer disc. However, as our simulations show, an additional layer of complexity is added when the small grains are dragged outwards by the gas, further accentuating isotopic variations in the disc. While backreaction can produce outward migration of small dust grains, viscosity is typically the dominant mechanism determining the radial velocities of the gas and small dust grains in the disc (Dipierro et al. 2018). Moreover, viscous migration is not restricted to regions of high dust-to-gas ratios so heterogeneities can occur across the entire disc. As such, we propose that viscosity plays a vital role in setting the isotopic variations in discs. Still other factors to consider are the radially decreasing surface density, which affects the rate of replenishment of silicate grains from the outer disc, and the propensity for presolar grains to merge with or break free from aggregates during collisions (not modelled here). All of these processes are summarised together in Figure 7.
4.2 Uncertainties in angular momentum transport

4.2.1 Lower or higher viscosity

Viscosity is one of the main drivers of the isotopic variations in our simulations. Although the nature of viscosity in discs is still not completely understood, accretion measurements of discs of different ages are consistent with some form of viscous evolution requiring the removal of angular momentum and transport of mass from the outer disc to the inner disc (e.g. King et al. 2007; Rafikov 2017). As molecular viscosity is far too weak to explain such measurements, it is usually assumed that viscosity originates from turbulence created by disc instabilities: magnetorotational (e.g. Balbus & Hawley 1991; Turner et al. 2014), gravitoturbulence (e.g. Gammie 2001; Rafikov 2015), and a host of hydrodynamic instabilities (e.g. Rossby wave, vertical shear, convective overstability, and zombie vortex; see Lyra & Umurhan 2019; and references therein). In the absence of non-magnetic turbulence, dead zones have been proposed to exist (Gammie 1996) near the disc mid-plane at radii $R \sim 1–10\,\text{au}$, where gas is not sufficiently ionised to sustain the magnetorotational instability. The presence of a dead zone would probably not affect the grain size distribution (or equivalently the isotopic concentrations) in the outer disc, but would almost certainly influence the inner disc. Diminished turbulence would produce smaller differential velocities between the dust, more efficient grain growth, less fragmentation, and marginal diffusion (Ciesla 2007; Brauer et al. 2008b). As a result, presolar grains would be rapidly swept up and locked away in larger aggregates, with little opportunity to produce isotopic variations because their dynamical mass would be so depleted.

Similar consequences may apply to discs where the global disc viscosity is low. The large number of phenomena contributing to the viscosity leads to a broad range in potential values for $\alpha_\text{SS} \in [10^{-4}, 0.04]$ (Rafikov 2017). Note our simulations sit roughly in the middle of this range (see Section 2.3.2). Reducing the viscosity by an order of magnitude would not only reduce the number of small dust grains in the disc by modifying the growth and fragmentation rates (e.g. transitioning from a fragmentation-limited to a drift-limited size distribution), it would also lower the outward radial velocity of the gas. Eventually, backreaction, which does not depend on viscosity, would take over as the dominant mechanism driving outward migration of gas and small dust grains in the disc.

Where and when backreaction dominates over viscosity depends on the local dust-to-gas ratio. Even in our moderately viscous simulations, we identified regions of our disc significantly altered by backreaction (Figure 2). In contrast, the component of the radial velocity due to backreaction at the beginning of our simulations, when the dust was still uniformly mixed, was only ~10% of the viscous component (see Appendix B in Dippiro et al. 2018; for a quantitative comparison under similar conditions). It is possible that backreaction can take over in driving isotopic variations in low viscosity environments, but probably on longer timescales and/or in limited regions of the disc where the dust-to-gas ratio and maximum grain size are higher. Even without backreaction, a non-zero differential velocity between the large and small grains (e.g. radial drift of large grains against a static background of small grains) could potentially generate variations. At the same time, a decrease in efficiency may also make the process more susceptible to disruption by grain growth, so further numerical experimentation is needed to say for sure.

While low disc viscosities are characteristic of more evolved discs, younger more massive discs can host viscosities that are much larger than what we consider in our simulations. If the disc is sufficiently massive, gravitoturbulence can trigger a dynamo that can amplify and sustain magnetic fields (Riols & Latter 2019) in a way that is resilient to the non-ideal magnetohydrodynamic (MHD) quenching effects of ohmic resistivity (Deng et al. 2020) and ambipolar diffusion (Riols et al. 2021). Under these conditions, the arguments made for the low viscosity regime can generally be reversed: more fragmentation, larger radial velocities, and stronger diffusion. In fact, diffusion in self-gravitating discs has been shown to homogenise spatial heterogeneities of passive isotopic tracers down to levels of ~10% (Boss 2008). These simulations provide a solid theoretical basis for starting our simulations from a homogeneous background of presolar grains, especially if discs start off more massive than assumed in the past (Schib et al. 2021). The corollary is that we cannot rely on inherited anisotropies to explain the origin of isotopic variations we find in the solar system and that evolutionary processes within the disc probably played a more central role. At the very least, we caution against qualitative descriptions of the disc phase without further exploring the variations that might arise from dynamics within the disc.
4.2.2 MHD winds and spiral density waves

Other non-diffusive forms of angular momentum transport are also relevant, such as MHD winds (Wardle & Koenigl 1993; Suzuki & Inutsuka 2009; Bai & Stone 2013) and spiral density waves (e.g. the leftmost panel in Figure 3). Wind-driven accretion from MHD winds occurs along a thin current layer near the disc’s surface, not too dissimilar to the flows we observe in the middle panel of Figure 3; however, in our simulations, these surface flows are a result of our locally isothermal equation of state and our inability to fully resolve the low-density surface layers of the disc. In reality, the surface of the disc is heated by irradiation from the central star and deviates from the local mid-plane isotherm. These warm, very diffuse surface layers are difficult to model with conventional SPH and, as a result, we lack some of the pressure support at the disc’s surface. Importantly, our results are not strongly biased by these surface flows due to their low densities. If anything, we would expect isotopic variations to be even stronger without these flows since they tend to homogenise the disc by transporting presolar grains back into the inner disc from whence they came. On the other hand, the presence of surface flows in our simulations shows that our results would not be significantly altered by MHD winds.

In real discs, the development of spiral density waves from an embedded planet, the planet’s migration through the disc, and the eventual opening of a gap are all gradual processes that span longer timescales than simulated in this study. To assess how presolar grains dynamically evolve in the presence of a giant planet we had to accelerate these processes by embedding a fully-formed, Jupiter-mass planet in our discs. However, this came at the cost of some of the realism. For example, the migration of the planet through the disc is initially much faster than a true Jupiter analogue due to the torques from co-orbital material that would no longer be present under realistic conditions. In fact, this rapid migration is partially responsible for the strong concentration of dust and resulting backreaction in the inner disc when the planet was initialised at 40 au (bottom panel of Figure 2). Although these conditions had some influence on the isotopic signatures observed in the inner disc, we nevertheless see the same trends inside of ~5 au for the other simulations in Figure 6 as well, despite the variety of dust concentrations. Thus we believe the trends to be real, even if the magnitudes may vary from reality. The isotopic variations in the outer disc are more robust because the mean radial velocity of the presolar grains is essentially the same with or without a planet present (rightmost panel in Figure 3).

4.2.3 Snow lines

Although not an angular momentum transport mechanism, snow lines similarly influence the radial drift of dust grains as they experience changes in size, composition, and morphology due to the freeze-out/sublimation of volatile elements on the grain’s surface. Changes to the stickiness and tensile strength of grains influence growth and fragmentation rates as a function of radius in the disc (e.g. Bogdan et al. 2020) and could lead to various trapping mechanisms (e.g. Pinilla et al. 2017; Vericel & Gonzalez 2020) that prevent the inward migration of dust from the outer disc. At the same time, fragmentation (Okuzumi et al. 2016) and/or breakup resulting from sublimation (Marov et al. 2021) could replenish the dynamic population of presolar grains that are transported radially outwards. Retention of large grains and replenishment of small grains near one or more snow lines could therefore be another important contributing factor to the build-up of isotopic variations in the disc (e.g. the shaded, downward-pointing arrow in Figure 7). Alternatively, if a snow line speeds up the loss of solids through radial migration (e.g. the arrow pointing to the left), then smoothing through homogenisation would be facilitated.

4.3 Comparison with meteorites

Meteorites come from bodies essentially found in the inner 10 au of the solar system. In Figure 6 we show data for solar system bodies measured from chondritic (enstatite, ordinary, and carbonaceous) and achondritic meteorites, as well as returned samples. Today’s orbit of Earth/Moon, Mars (the parent body of shergottites, nakhlites, and chassignites; SNC), and Vesta (the most likely parent body for howardites, eucrites, and diogenite; HED) are well known: [1, 1.52, 2.36] au. However, while chondritic asteroids are observed mainly in the asteroid belt, it is unlikely that this was their original location. ECs display isotopic compositions close to the Earth-Moon system in many isotopic systems (e.g. Javoy et al. 2010) such as O (Clayton et al. 1984), Cr (Trinquier et al. 2007), and Ti (Trinquier et al. 2009). These similar compositions place their original location in the same region as Earth (placed at 1.2 au for clarity). It is worth pointing out that some isotopic systems, notably $\delta^{30}$Si (Fitoussi & Bourdon 2012), display compositions distinct from that of the Earth, although the Si isotope anomalies are not of nucleosynthetic origin. It has been argued that these deviations are most likely due to processes linked to silicate-metal partition during planetary differentiation (e.g. Fitoussi et al. 2009) or nebular processes in reductive conditions close to the Sun (Sikdar & Rai 2020; Dauphas et al. 2015). OCs have been placed at the location of the inner part of the asteroid belt (2.2 au). Multiple lines of evidence suggest that CCs formed further out than ECs and OCs (e.g. Warren 2011). They have higher water content than other chondritic groups (Alexander et al. 2012), placing their formation region further out in the disc. For ease, we place the markers at modern-day Jupiter (5.2 au), but note there is a wide spread in formation radii between subgroups (especially for CI and metal-rich CCs; see Desch et al. 2018; van Kooten et al. 2020). CCs also show distinct isotopic compositions from OCs and ECs in many isotopic systems, such as $\varepsilon^{56}$Mo, $\varepsilon^{186}$Os, and $\varepsilon^{110}$Pd (Ek et al. 2020) or $\varepsilon^{50}$Ti and $\varepsilon^{54}$Cr (Trinquier et al. 2007; Leya et al. 2008; Trinquier et al. 2009).

Although our simulations suffer from low resolution in the inner disc, we observe clear variations within $R \lesssim 5$ au in every simulation for all three isotopic systems considered in our study (Figure 6). Here the enrichment in presolar grains relative to the larger silectites with ISM compositions is partially due to the faster migration rates of larger grains (resulting in increased accretion onto the central star) and partially due to the lack of confinement of small grains in dust traps (whether self-induced or in pressure bumps at disc/gap edges). The inner regions of real discs are dynamically more complex and likely to be case dependent; however, even as a first-order estimate, this result is significant because it implies that disc dynamics may have had an in situ role in determining the isotopic composition of meteorite parent bodies.

It should also be remembered that the magnitude of the isotopic variations in our simulations depends on the initial conditions of our model, such as: the number of presolar grain types, their grain-size distribution, the type and amount of isotopic tracers they carry, and whether or not presolar grains are included in the makeup of larger aggregates. We constrained these initial conditions using presolar grain data obtained from the meteorite record (see Section 2.4.1), but because of the limited constraints available on the initial fraction of presolar grains in the disc that may also be locked up in larger aggregates, we resorted to modelling two extreme scenarios:
our so-called dynamical and aggregate cases (see Section 2.2.3).
In the aggregate case, more than 97% of presolar grains were homogeneously mixed into the silicate population. This mitigated the enrichment of presolar grains through disc evolution by reducing the available mass that could move relative to the larger silicates. Even with $\lesssim 3\%$ of presolar grains remaining in the dynamical mass, the aggregate case was far closer to typical solar system values for the three isotopic systems we considered (bottom panels in Figure 6). Note, for example, the similar magnitudes in the peaks around the planet for $^{54}\text{Cr}$ and $^{50}\text{Ti}$ to those measured in CCs (Trinquier et al. 2009, 2007; Gerber et al. 2017). Although we expect grain growth to reduce the concentration efficiency of presolar grains in our simulations, this is counterbalanced by the $\gtrsim 100\%$ longer timescales over which isotopic anomalies can develop in real discs compared to what we have simulated here. Therefore, at any given time, the disc only needs a small fraction of presolar grains to be dynamically independent of the silicate population in order for this mechanism to work. It is plausible that such a small fraction of presolar grains could be continuously maintained by either fragmentation or infall.

In addition to the magnitude of the profile features in Figure 6, the trends common to each simulation share some intriguing similarities with solar system material (although, given the many differences between our model and the actual solar system, care should be taken not to over interpret these results). Solar system measurements of objects from the Sun to the location of 4-Vesta in the asteroid belt exhibit a negative gradient in $^{54}\text{Cr}$ and $^{50}\text{Ti}$ (a positive gradient for $^{96}\text{Zr}$), features that are mirrored in our no-planet simulation. The simulations with embedded planets also exhibit a general decline (resp. incline) towards intermediate radii, but the variations are muted relative to the no-planet case and more rounded-flat near $\sim 1\text{ au}$.

The strong gradients we see in the outer regions of our simulations are also of great interest, since local variations can be inherited by growing aggregates that migrate in and get trapped at the outer edge of the gap carved by the planet. Such a scenario could contribute to the sudden increase and/or variation (e.g. from pebbles formed at different radii or times) in isotopic ratios measured in CCs that are thought to have originated beyond Jupiter’s orbit.

This predicted enrichment of presolar grains in the outer disc is also consistent with the greater abundance of presolar grains found in cometary matter ($\sim 600$–$1100$ ppm Floss et al. 2013; Leitner et al. 2012) and interplanetary dust particles (Floss et al. 2006; Davidson et al. 2012; Busemann et al. 2009; Croux et al. 2015) versus chondrites ($\sim 200$ ppm Floss & Haenecour 2016). While promising, this explanation of events does not explain the variations created from these processes can be continuously reinforced throughout the evolution of the disc. This is in contrast to variations inherited from the parent molecular cloud only during the early (Class 0/I) phases of the disc’s history. Evidence from the literature suggests that turbulence during these younger, more massive phases would have been particularly efficient at homogenising inherited presolar grain populations. Our simulations additionally show that diffusive mixing is further facilitated by rapid accretion flows near the disc’s surface (e.g. due to magnetically induced winds) in order to explain these observations. However, it is difficult to say more without (i) having a dedicated model of the solar system, (ii) accounting for the other shortcomings of our model and (iii) having more Zr isotope data available for other presolar grains (e.g. silicates).

Still yet another uncertainty is how far out these isotopic variations are still relevant for solar system bodies. Note the decreasing density with radius is, at least in part, compensated by the increasing isotopic variation. Thus, supposing that the initial circumsolar disc extended to hundreds of au, it is possible that size sorting of presolar grains in the outer disc could still be relevant (e.g. the feature at $R \sim 170$ au in the rightmost column of Figure 6 caused by the larger SiC grains stalling earlier than oxide grains in the viscous expansion of the disc). At these distances, however, external photo-evaporation caused by irradiation from nearby stars could truncate the disc (e.g. Facchini et al. 2016; Haworth et al. 2017) and remove presolar grains (particularly the smaller oxide grains) from the system. Similarly uncertain is the importance of the peak immediately surrounding the planet. This peak is clearly associated with the low-density gap created by the planet, where, due to interactions with the gas, the large grains are highly depleted relative to the small grains (see Figure 2 and associated text). Here the particle crossing times may be too fast (see Figure 4) for any meaningful signature to develop out of this region of the disc. Long term studies including grain growth and fragmentation would be needed to assess the importance of these regions further.

5 CONCLUSIONS
There is a sizeable body of literature on the dynamics and transport of dust in protoplanetary discs, but little has been done to quantitatively connect the dynamics from these models to presolar grains and the nucleosynthetic variations they may have produced in early solar system bodies. To better bridge this gap, we conducted a series of 3D, gas-dust SPH simulations of a viscous protoplanetary disc containing 17 dust phases that span two presolar grain populations (oxide and silicon carbide) and one aggregate population (solar system silicates). We additionally explored the effect of inserting a massive planet at different locations in the disc as well as increasing the overall dust-to-gas ratio. For each scenario, we ran corresponding “single-grain” simulations for eight of the 17 dust phases in order to isolate the effects of backreaction from viscosity and to assess how backreaction affects grains of different sizes. Finally, we calculated isotopic ratios for $^{54}\text{Cr}$ (carried by oxide grains), $^{96}\text{Zr}$ (carried by silicon carbide grains), and $^{50}\text{Ti}$ (carried in both presolar types) using the resulting surface densities for the dust and assuming presolar grains were either distinct from the solar system silicates (dynamical case) or partially mixed within silicates greater than $10\mu\text{m}$ (aggregate case).

The main conclusion from our study is that nucleosynthetic variations arise naturally due to viscosity and drag – two fundamental processes of protoplanetary disc evolution. As such, variations created from these processes can be continuously reinforced throughout the evolution of the disc. This is in contrast to variations inherited from the parent molecular cloud only during the early (Class 0/I) phases of the disc’s history. Evidence from the literature suggests that turbulence during these younger, more massive phases would have been particularly efficient at homogenising inherited presolar grain populations. Our simulations additionally show that diffusive mixing is further facilitated by rapid accretion flows near the disc’s surface (e.g. due to magnetically induced winds)
and dynamical interactions with planets. Importantly, the variations we observe in our simulations operate despite this homogenisation. Even in low-viscosity environments (e.g. dead zones or late evolutionary stages), isotopic variations can still be generated through backreaction and/or dilution from large silicate aggregates that accumulate in the inner disc due to radial migration. We therefore caution that dust dynamics within the circumstellar disc should not be neglected when addressing the origins of isotopic variations in the solar system. We further emphasise that it is not enough to simulate presolar grains on their own, but that it is the joint evolution of both small and large dust populations that gives rise to the nucleosynthetic variations in our simulations.

Other key results can be summarised as follows:

(i) Viscous expansion is more efficient than backreaction at driving the outward migration of presolar dust grains, except in regions where the local dust-to-gas ratio exceeds $\kappa \gtrsim 0.1$.

(ii) The outer disc is preferentially enriched with presolar grains due to the net outward migration of small dust grains and inward migration of large silicate grains. Aggregates that grow from this enriched material will either fragment and be recycled in the outer disc or migrate in and get caught in dust traps (e.g. the outer edge of the gap carved by Jupiter). The latter could potentially account for some of the differences in isotopic ratios found in carbonaceous chondrites relative to enstatite and ordinary chondrites found closer to the Sun.

(iii) Size/density sorting of presolar grains only occurs in the far outer regions of the disc undergoing viscous expansion. The larger silicon-carbide grains are the first to stall in the outflow, leaving the disc beyond $R \gtrsim 200$ au enriched in oxides.

(iv) At any given time, only a small fraction of the presolar grain population (e.g. maintained by fragmentation or infall) needs to be dynamically independent of solar system silicates in order for isotopic variations to develop.

(v) A giant planet only influences the net radial migration rates of presolar grains interior to its own orbit. While planet migration can scatter presolar grains into the outer disc, the gap the planet carves prevents radial surface flows from carrying these grains back into the inner disc (although small dust grains are still able to cross the gap at the mid-plane due to viscous diffusion and spiral density waves).

The biggest shortcoming of our model is the lack of grain growth and fragmentation in our dust populations, which may taint our results. To mitigate these effects we have limited ourselves to simulating short evolutionary timescales; however, future work is needed to explore how grain growth and fragmentation affect presolar grain dynamics over longer timescales and under conditions more representative of the early solar system. Due to the close dynamical link between the presolar grains and the gas, constraints on the dynamical history of presolar grains could give us more insight into the viscous evolution of the early solar system.

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DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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APPENDIX A: ARCSINE INTERPOLANT

A1 Motivation

To date there have been three different parameterisations of the dust-to-gas ratio used in the one-fluid literature. (i) First was the so-called dust fraction, \( \epsilon \equiv \rho_d/\rho = \epsilon/(1-\epsilon) \), introduced by Laibe & Price (2015) to avoid a singularity in the one-fluid equations when \( \rho_d = 0 \). Although it soon became apparent that the one-fluid method was ill-suited for gas-poor environments, \( \epsilon \) continued to be a convenient parameterisation for future derivations. (ii) Secondly, \( S = \sqrt{\pi \epsilon} \) was used by Price & Laibe (2015) to prevent negative dust masses from occurring. While evolving \( S \) enforced the physical condition \( \epsilon < 0 \), it did nothing to prevent the equally unphysical situation \( \epsilon > 1 \). (iii) Finally, Ballabio et al. (2018) proposed parameterising the dust-to-gas ratio directly using \( S = \sin \theta \), or equivalently \( \epsilon = \sin^2 \theta \). This last method not only enforced the physical conditions \( \epsilon \in [0,1] \), or equivalently \( \epsilon \in [0,\infty) \), but improved the general accuracy of the one-fluid method during benchmarking tests. The only negative aspect about \( S \) were its continued to be a convenient parameterisation for future derivations. (ii) Secondly, \( S = \sqrt{\pi \epsilon} \) was used by Price & Laibe (2015) to prevent negative dust masses from occurring. While evolving \( S \) enforced the physical condition \( \epsilon < 0 \), it did nothing to prevent the equally unphysical situation \( \epsilon > 1 \). (iii) Finally, Ballabio et al. (2018) proposed parameterising the dust-to-gas ratio directly using \( S = \sin \theta \), or equivalently \( \epsilon = \sin^2 \theta \). This last method not only enforced the physical conditions \( \epsilon \in [0,1] \), or equivalently \( \epsilon \in [0,\infty) \), but improved the general accuracy of the one-fluid method during benchmarking tests. The only negative aspect about \( S \) were its

\[ \theta \equiv \sin^{-1} \sqrt{\epsilon} \quad \text{or} \quad \epsilon = \sin^2 \theta, \quad (A1) \]

which was attractive because it gave the same functional form as \( S \) at low dust fractions (since \( \theta \ll 1 \) implies \( \epsilon \sim \theta^2 \)) where \( S \) performed superior to \( \theta \). Furthermore, Equation (A1) automatically enforced

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APPENDIX A: ARCSINE INTERPOLANT

A1 Motivation

To date there have been three different parameterisations of the dust-to-gas ratio used in the one-fluid literature. (i) First was the so-called dust fraction, \( \epsilon \equiv \rho_d/\rho = \epsilon/(1-\epsilon) \), introduced by Laibe & Price (2015) to avoid a singularity in the one-fluid equations when \( \rho_d = 0 \). Although it soon became apparent that the one-fluid method was ill-suited for gas-poor environments, \( \epsilon \) continued to be a convenient parameterisation for future derivations. (ii) Secondly, \( S = \sqrt{\pi \epsilon} \) was used by Price & Laibe (2015) to prevent negative dust masses from occurring. While evolving \( S \) enforced the physical condition \( \epsilon < 0 \), it did nothing to prevent the equally unphysical situation \( \epsilon > 1 \). (iii) Finally, Ballabio et al. (2018) proposed parameterising the dust-to-gas ratio directly using \( S = \sin \theta \), or equivalently \( \epsilon = \sin^2 \theta \). This last method not only enforced the physical conditions \( \epsilon \in [0,1] \), or equivalently \( \epsilon \in [0,\infty) \), but improved the general accuracy of the one-fluid method during benchmarking tests. The only negative aspect about using \( S \) over \( \theta \) is the increase in dispersion of the dust-to-gas ratio along steep dust gradients that could potentially drive instabilities in low-density regions.

In this paper we used a parameterisation of the dust-to-gas ratio proposed by G. Laibe (private communication):

\[ \theta \equiv \sin^{-1} \sqrt{\epsilon} \quad \text{or} \quad \epsilon = \sin^2 \theta, \quad (A1) \]

which was attractive because it gave the same functional form as \( S \) at low dust fractions (since \( \theta \ll 1 \) implies \( \epsilon \sim \theta^2 \)) where \( S \) performed superior to \( \theta \). Furthermore, Equation (A1) automatically enforced
the same physical constrains as \( \tilde{S} \). Indeed, during testing we found that \( \theta \) captured the best qualities of both \( S \) and \( \tilde{S} \), including the increased accuracy. However, we also found that the trigonometric functions produced a noticeable overhead that resulted in longer computation times.

\section*{A2 Continuum equations}

The local conservation of the dust mass is given by

\[
\frac{d\rho}{dt} = -\frac{1}{\rho} \nabla \cdot \left[ \epsilon (1 - \epsilon) \rho \Delta V \right],
\]

where \( \Delta V = v_d - v_g \) is the differential velocity between the gas and the dust. In the terminal velocity approximation, when the only source of differential acceleration is the gas pressure gradient, Equation (A2) reduces to

\[
\frac{d\rho}{dt} = -\frac{1}{\rho} \nabla \cdot ( \epsilon \tau \nabla P ).
\]

Substituting Equation (A1) into Equation (A3), the evolution equation for \( \theta \) becomes

\[
\frac{d\theta}{dt} = -\frac{1}{2\rho \sin \theta \cos \theta} \nabla \cdot \left( \sin^2 \theta \nabla P \right).
\]

\section*{A3 Discretisation}

\subsection*{A3.1 Standard method}

Using the standard SPH interpolation scheme (see Equation 93 of Price 2012),

\[
\sum_b m_b f_b \left( \kappa + \epsilon \right) (A_a - A_b) \frac{\hat{F}_{ab}}{|r_{ab}|} \approx \frac{1}{\rho f} \nabla \cdot \left( \rho f^2 \kappa \nabla A \right),
\]

we obtain the SPH version of Equation (A4) by setting \( A = P \), \( f = \sin \theta \cos \theta \), and \( \kappa = \sin^2 \theta \rho \cos^2 \theta \):

\[
\frac{d\hat{F}_{ab}}{dt} = -\frac{1}{2\rho \sin \theta \cos \theta} \sum_b m_b \sin \theta_b \cos \theta_b \left( \frac{\hat{F}_{ab}}{|r_{ab}|} \right) (P_a - P_b).
\]

Here and in what follows, subscripts \( a \) and \( b \) are particle indices, \( r_{ab} \) is the distance between particles (or a unit vector if boldface and wearing a hat), \( F_{ab} \) is the scalar part of the kernel gradient (i.e. \( \nabla_a W_{ab} = F_{ab} \hat{r}_{ab} \), where \( W \) is the smoothing kernel), and \( \hat{F}_{ab} = \frac{1}{2} \left[ F_{ab}(h_a) + F_{ab}(h_b) \right] \), where \( h \) is the SPH smoothing length.

While Equation (A6) ensures exact conservation of total dust mass, it is prone to numerical instabilities at low dust fraction. Despite \( \theta_{a,b} \approx 0 \), they both typically remain finite and the ratio \( \sin \theta_b / \sin \theta_a \sim \theta_b / \theta_a \) varies wildly among neighbours. Hutchison et al. (2016) experienced a similar issue in their full one-fluid equations (i.e. without the terminal velocity approximation), which they solved by violating conservation properties and removing the offending ratio for their equations. Since conservation is one of the big advantages to using SPH, we wished to look for an alternate mass-conserving discretisation where this factor simply does not occur.

\subsection*{A3.2 Stable method}

A hint at a possible solution comes from temporarily ignoring particle indices on \( \theta \) in Equation (A7), canceling like terms, and finally rearranging and assigning indices so as to preserve the symmetry between particle pairs:

\[
\frac{d\theta_{ab}}{dt} = -\frac{1}{\sin 2\theta_{ab}} \sum_b m_b \frac{\sin \theta_a \sin \theta_b}{P_a - P_b} \frac{\hat{T}_{ab}}{|r_{ab}|},
\]

where we have intentionally preserved the \( \sin \theta_{ab} \) term in the numerator to emphasise the particle symmetry (despite formally canceling out upon expanding \( \sin 2\theta_0 = 2 \sin \theta_0 \cos \theta_0 \)). A singularity remains at \( \theta_0 = \pi / 2 \) (\( e = 1 \)); however, the same is true for the \( \tilde{S} \) parameterisation, and the terminal velocity approximation would break down long before this limit could be reached anyway.

Given the cavalier approach we took in building Equation (A7), it is not immediately obvious that Equation (A7) is a valid discretisation for Equation (A3). Its validity can be shown by following the procedure laid out in Appendix A of Price & Laibe (2015). We begin by introducing a new kernel function

\[
\nabla^2 \tilde{Y}_{ab} \equiv -\frac{\hat{T}_{ab}}{|r_{ab}|},
\]

such that the Laplacian of the standard SPH summation interpolant is

\[
\nabla^2 \tilde{A}_{ab} \approx \sum_b \frac{m_b}{\rho_b} \tilde{Y}_{ab}.
\]

Rewriting Equation (A7) in the form

\[
\frac{d\theta_{ab}}{dt} = -\frac{1}{\rho_a \sin \theta_a \cos \theta_a} \sum_b \frac{m_b}{\rho_b} \left( D_a + D_b \right) \left( P_a - P_b \right) \nabla^2 \tilde{Y}_{ab},
\]

where \( D_a = \sin \theta_a \sin \theta_b \sin t_{a,b} \) and \( D_b = \sin \theta_a \sin \theta_b \sin t_{b,a} \), we can then expand the equation to

\[
\frac{d\theta_{ab}}{dt} = -\frac{1}{2\rho_a \sin \theta_a \cos \theta_a} \sum_b \frac{m_b}{\rho_b} \left[ P_a (D_a - D_b) - P_b (D_a - D_b) \right].
\]

Transforming each term according to Equation (A9) and simplifying using the identity

\[
\nabla^2 \left( P \nabla \right) = \rho \nabla^2 P - \rho \nabla \cdot \left( \nabla P \cdot \nabla \right) - \Delta P \nabla^2 \left( \nabla \right),
\]

we obtain

\[
\frac{d\theta}{dt} = -\frac{1}{\rho} \sin 2\theta \left( \rho \nabla^2 \left( \nabla \right) + \nabla \cdot \left( \nabla \cdot \nabla \right) \right),
\]

\[
= -\frac{1}{\rho} \sin 2\theta \nabla \cdot \left( \nabla \left( \nabla \cdot \nabla \right) \right),
\]

which is the continuum equation in Equation (A4), thus establishing the validity of Equation (A7).

\section*{A4 Conservation}

Although the previous section proves the viability of Equation (A7), it does not guarantee that it will conserve mass and energy when combined with the other fluid equations.
A4.1 Mass

In SPH, total mass is exactly conserved by virtue of the fixed particle masses. This is also true in the one-fluid formalism, but the dust mass ($M_d = \sum_a m_a \sin^2 \theta_a$) depends crucially on the evolved quantity $\theta$. Therefore any conservative SPH scheme must satisfy the relation

$$\frac{dM_d}{dt} = \sum_a m_a \cos \theta_a \sin \theta_a \frac{d\theta_a}{dt} = 0.$$  \hfill (A14)

After expanding $\frac{d\theta_a}{dt}$ using Equation (A7), the previous relation becomes

$$\sum_a \sum_b m_a m_b \sin \theta_a \sin \theta_b (t_{s,a} + t_{s,b}) (P_a - P_b) \frac{\bar{T}_{ab}}{|v_{ab}|} = 0.$$  \hfill (A15)

Noting that $\bar{T}_{ab} = \bar{T}_{ba}$ and $|v_{ab}| = |v_{ba}|$, it is easy to see that Equation (A15) is true by (i) swapping the summation indices in the double sum and (ii) adding half of the original term to half of the rearranged term, giving zero.

A4.2 Energy

With the new $\theta$ parameterisation, the energy of the system can be written as

$$E = \sum_a m_a \left[ \frac{1}{2} \dot{v}_a^2 + u_a \cos^2 \theta_a \right],$$  \hfill (A16)

which is conserved if

$$\frac{dE}{dt} = \sum_a m_a \left[ \dot{v}_a \frac{dv_a}{dt} + \cos^2 \theta_a \frac{du_a}{dt} - 2 u_a \sin \theta_a \cos \theta_a \frac{d\theta_a}{dt} \right] = 0.$$  \hfill (A17)

Removing all of the non-dust components from the above relation (assuming energy is conserving) leaves

$$\frac{dE}{dt} \bigg|_{\text{dust}} = \sum_a m_a \cos^2 \theta_a \frac{du_a}{dt} \bigg|_{\text{dust}} + \sum_a \sum_b m_a m_b u_a \sin \theta_a \sin \theta_b \frac{\rho_a \rho_b}{\rho_a \rho_b} (t_{s,a} + t_{s,b}) (P_a - P_b) \frac{\bar{T}_{ab}}{|v_{ab}|} = 0.$$  \hfill (A18)

Swapping the indices of the term with two summations and adding half of the original term to half of the rearranged term, we can then directly solve for the energy conserving form of the internal energy:

$$\frac{du_a}{dt} \bigg|_{\text{dust}} = - \frac{1}{2 \cos^2 \theta_a} \sum_b m_b \sin \theta_a \sin \theta_b \left( (t_{s,a} + t_{s,b}) (P_a - P_b) \frac{\bar{T}_{ab}}{|v_{ab}|} \right).$$  \hfill (A19)

A5 Multigrain

The multigrain equations are also straightforward to derive by exchanging $\epsilon \rightarrow \epsilon_j$ and $\theta \rightarrow \theta_j$ in Equation (A1) and subsequent equations. In particular, Equation (A4) becomes

$$\frac{d\theta_j}{dt} = \frac{1}{2 \sin \theta_j} \frac{d\epsilon_j}{dt}.$$  \hfill (A20)

Table B1. Table summarising the elemental concentrations, isotopic abundances, and isotopic ratios used for mass balance calculations.

| Concentrations (ppm) | Isotopic abundances | Isotopic ratios d-e |
|----------------------|---------------------|---------------------|
| C/O/SiO | 2645.7 h^4Ti/Ox | 0.378444 (h^4Ti/Ox/Cr) | 0.098920 |
| C/O/SiC | 23180.8 h^4Si/Ox | 0.711235 (h^4Si/Ox/Cr) | 0.082445 |
| Zn/Zr | 3.7 h^4Zr/Ox | 0.10916 (h^4Zr/Ox/Zr) | 0.46813 |
| Zn/Zr | 25.0 h^4Zr/Ex | 0.18637 (h^4Zr/Ex/Zr) | 0.970501 |
| Ti/Ti | 445.3 h^4Ti/Ex | 0.738079 (h^4Ti/Ex/Ti) | 0.072511 |
| Ti/Ti | 20390.0 h^4Ti/Ex | 0.432627 (h^4Ti/Ex/Ti) | 0.086867 |
| Ti/Ti | 24.4 h^4Ti/Ex | 0.437008 (h^4Ti/Ex/Ti) | 0.086415 |

\footnotesize

* Concentrations of elements are given in ppm (part per million) for bulk-rock CI (Barrett et al. 2012) to represent solar system silicates. Concentrations for presolar SiC and Oxides from Kasri et al. (2001; Amari et al. (1995; and Zega & et al. (2014), respectively.

\footnotesize

* Isotopic abundance of most abundant isotope of associated element used to calculate isotopic ratios with rare isotope. Calculated using terrestrial and presolar grains values from references below.

\footnotesize

* Isotopic ratios for presolar SiC and oxides from the Presolar Grain Database (Hynes & Gyngard 2009), except for Ti isotopic ratios (h^4Ti/Ox/Cr) from Nittler et al. (2018), DuPasquier et al. (2019), Qin et al. (2021).

\footnotesize

* Isotopic ratios for solar system silicates from Trinquier et al. (2009) for h^4Ti/Ox, Schönbuchler et al. (2004) for h^4Zr/Zr, Leya et al. (2007) for h^4Ti/Ti.

where from Hutchison et al. (2018) we know that

$$\frac{d\epsilon_j}{dt} = - \frac{1}{\rho} \cdot \left[ \epsilon_j \left( \sum_k \frac{\epsilon_k}{\sum_{L_k}} \right) \nabla P \right].$$  \hfill (A21)

The resulting continuum form for the multigrain case can then be written as

$$\frac{d\theta_j}{dt} = - \frac{1}{2 \rho \sin \theta_j} \cdot \left[ \sin^2 \theta_j T_{s,j} \nabla P \right],$$  \hfill (A22)

where

$$T_{s,j} = \left( \sum_k \frac{\epsilon_k}{\sum_{L_k}} \right).$$

Because the form of Equation (A22) is the same as in the single-fluid case, we can jump straight to the discretised version

$$\frac{d\theta_j}{dt} = - \frac{1}{\sin \theta_j} \sum_b m_b \frac{\sin \theta_j \sin \theta_j}{\rho_a \rho_b} \left( T_{s,j,a} + T_{s,j,b} (P_a - P_b) \frac{\bar{T}_{ab}}{|v_{ab}|} \right).$$  \hfill (A23)

Similarly, the energy equation retains the same form as the single-phase only with the stopping time replaced by $T_{s,j}$:

$$\frac{du_a}{dt} \bigg|_{\text{dust}} = - \frac{1}{2 \cos^2 \theta_a} \sum_b m_b \frac{\sin \theta_j \sin \theta_j}{\rho_a \rho_b} \left( T_{s,j,a} + T_{s,j,b} (P_a - P_b) (u_a - u_b) \frac{\bar{T}_{ab}}{|v_{ab}|} \right).$$  \hfill (A24)

APPENDIX B: INPUT FOR MASS BALANCE CALCULATIONS

The data used for mass balance calculations presented in Section 2.4.2 are summarised in Table B1. Solar system silicate grains are approximated to CI chondrite compositions in terms of elemental concentrations (Barrat et al. 2012) and to terrestrial values for isotopic ratios (Leya et al. 2007; Schönbuchler et al. 2004; Trinquier et al. 2009).

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