Size and density sorting of dust grains in SPH simulations of protoplanetary discs

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Accepted 2017 March 30. Received 2017 March 30; in original form 2016 May 10.

ABSTRACT

The size and density of dust grains determine their response to gas drag in protoplanetary discs. Aerodynamical (size×density) sorting is one of the proposed mechanisms to explain the grain properties and chemical fractionation of chondrites. However, the efficiency of aerodynamical sorting and the location in the disc in which it could occur are still unknown. Although the effects of grain sizes and growth in discs have been widely studied, a simultaneous analysis including dust composition is missing. In this work we present the dynamical evolution and growth of multicomponent dust in a protoplanetary disc using a 3D, two-fluid (gas+dust) Smoothed Particle Hydrodynamics (SPH) code.

We find that the dust vertical settling is characterised by two phases: a density-driven phase which leads to a vertical chemical sorting of dust and a size-driven phase which enhances the amount of lighter material in the midplane. We also see an efficient radial chemical sorting of the dust at large scales. We find that dust particles are aerodynamically sorted in the inner disc. The disc becomes sub-solar in its Fe/Si ratio on the surface since the early stage of evolution but sub-solar Fe/Si can be also found in the outer disc-midplane at late stages.

Aggregates in the disc mimic the physical and chemical properties of chondrites, suggesting that aerodynamical sorting played an important role in determining their final structure.

Key words: protoplanetary discs — methods: numerical — astrochemistry — meteorites, meteors, meteoroids

1 INTRODUCTION

In protoplanetary discs the interaction between gas and dust plays a central role in determining the dust dynamics. The settling and drift of a dust particle due to the aerodynamic drag exerted by the surrounding gas is driven by the size and the density of the considered particle and, thus, by the stopping time,

\[ t_s = \frac{\rho_d s_d^2}{c_s \rho_g} \]  

(1)

where \( s_d \) is the size (radius) of the particle, \( \rho_d \) its intrinsic density, \( c_s \) the sound speed, and \( \rho_g \) the gas density (Weidenschilling 1977). As such, for a given set of parameters \((c_s, \rho_g)\), the dynamical behaviour of the particle is determined by the product of size and density, which is called the aerodynamic parameter (Cuzzi & Weidenschilling 2006), \( \zeta = \rho_d s_d \): smaller and lighter particles have short stopping times and are well coupled to the gas while larger and denser grains have longer stopping times and are less coupled to the surrounding gas.

Furthermore, the rate of radial drift of a particle reaches its maximum when \( t_s/t_{orb} = 1/2\pi \) (Weidenschilling 1977), where \( t_{orb} \) is the orbital period

\[ t_{orb} = \frac{2\pi}{\Omega_k} \]  

(2)

Thus, combining the stopping time, equation (1), with the orbital period, the optimal drift size for a given species, corresponding to the fastest drift rate, \( s_{opt} \), can be derived:

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arXiv:1703.10385v1 [astro-ph.EP] 30 Mar 2017
Equation 3 states that for given conditions, the optimal drift size varies with the intrinsic density of the considered dust particle. Moreover, the value of $s_{\text{opt}}$ in the midplane, $s_{\text{mid, opt}}$, can be written as

$$s_{\text{mid, opt}} = \frac{\Sigma_g}{2 \pi \rho_d},$$

where $\Sigma_g$ is the gas surface density. The dependence of $s_{\text{opt}}$ on the particle intrinsic density is also evident.

The different response to the gas drag of dusty aggregates with different sizes and densities is thought to have contributed to the determination of the physical and chemical properties of the pristine complex aggregates in our early Solar System: chondrites (Scott & Krot 2003; Cuzzi & Weidenschilling 2006). Chondrites host other components: (i) calcium-aluminum rich inclusion (CAIs), made of refractory material, (ii) amoeboid olivine aggregates, characterized by fine olivine grains, metals and refractory compounds, (iii) metallic grains (Fe-Ni), and (iv) matrix, an unequilibrated volatile-rich mixture (MacPherson 2003; Scott & Krot 2003; Scott 2007). Chondrites are among the oldest rocks known. They retain radiometric ages corresponding to the first few Myr after calcium–aluminum rich inclusions (whose formation dates at 4567.2 ± 0.6 Myr ago (Amelin et al. 2002)), and thus record events that occurred at the beginning of the Solar System formation.

The formation of chondrules was an ongoing process which occurred from the formation of CAIs and lasted 3 Myr (Connelly et al. 2012). The size of chondrules varies within each clan as well as between different chondrite groups (Rubin 2010), see Fig. 1. There is a general size-density correspondence between chondrules, metallic grains (Fe-Ni) and sulfide grains, within the same group of chondrites, for which $(\rho_s)_{\text{chond}} \sim (\rho_s)_{\text{metal}} \sim (\rho_s)_{\text{sulf}}$ (Benoit et al. 1998; Kuebler et al. 1999). Size sorting and size-density sorting due to gas drag in different scenarios (local turbulences, large disc scale turbulences, jet-flow) are some of the proposed mechanisms to explain the chondrule size distribution, the assemblage of the chondrite components, and the size-density correspondence between chondrules, metallic grains (Fe-Ni) and sulfide grains, within the same group of chondrites (Clayton 1980; Benoit et al. 1998; Kuebler et al. 1999; Cuzzi et al. 2001; Liffman 2005; Zanda et al. 2006; Jacquet et al. 2012).

Chondrites exhibit different degrees of elemental fractionation, for example in their metal-silicate content (Larimer & Anders 1970). The Fe/Si ratio of chondrites normalized to CI chondrites (whose Fe/Si ratio is close to the solar value) varies according to the chondrites group (Palme & Jones 2003; Scott & Krot 2005), see Fig. 2. Moreover the ratio of oxidized iron and metallic iron+sulfides to silicon, changes for different chondrite groups, Fig. 3. The chemical and physical properties of chondrites suggest that chondrites formed, accreted and evolved in distinct disc regions and at different times, within different chemical reservoirs (Scott & Krot 2005).

Aerodynamic sorting, photophoresis, magnetic properties, grain aggregation, and heating processes, both in large (disc, eddies) and small (chondritic parent bodies) scales, are among the suggested theories to produce the observed trend (Larimer & Wasson 1988a,b; Moore et al. 2003; Wurm et al. 2013; Cuello et al. 2016). However, the level of contribution of dynamical sorting in assembling the chondritic material is not well constrained (Rubin 2010).

Size sorting of dust has been observed in protoplanetary discs. Pinte et al. (2007) modeled the dust size distribution for GG Tau, a circumbinary disc, finding that multiple populations of dust, each with different sizes and scale heights, are necessary to match the observed brightness profile. They found that 1 $\mu$m, 2.5$\mu$m, 5$\mu$m, 7.5$\mu$m, 10$\mu$m grains have a decreasing scale height suggesting a stratified structure of
the dust. Another T-Tauri object which shows dust sorting is TW Hya. TW Hya has been widely studied at different wavelengths, each probing different dust sizes (Wilner et al. 2000, 2003; Hughes et al. 2007, 2008; Andrews et al. 2012; Menu et al. 2014). All observations suggest that vertical and radial sorting of the dust is efficient in TW Hya: the abundance of larger grains peaks at the midplane and in the inner radial regions while smaller grains encompass the larger grains occupying large radial distances and vertical extension of the disc. Thus, observation suggests that sorting is a process which characterizes the dust dynamics at very large disc scales.

Several studies in the past investigated the vertical settling and radial drift of grains as a function of their size (Dullemond & Dominik 2004; Barrière-Fouchet et al. 2005; Dullemond & Dominik 2008; Ciesla 2009), and in the resulting observational properties of discs (Dullemond & Dominik 2004). An extensive review of the processes involved in gas-dust dynamics and interactions has been made by Cuzzi & Weidenschilling (2006).

In addition, the early stage of planet formation is characterized by a fast growth of submicron-size grains to large planetesimals (Dominik et al. 2007). Signatures of rapid grain growth have been extensively found in protoplanetary discs from observations at different wavelengths (Throop et al. 2001; Testi et al. 2003; Bouwman et al. 2008; Ubach et al. 2012). The growth of grains is a complex process which involves, beside the physical conditions of the disc, the chemical and physical properties of the dust (Ormel et al. 2007; Blum & Wurm 2008; Okuzumi et al. 2012). Moreover, collisions of grains do not always produce perfect sticking and fragmentation and bouncing of grains upon collisions can occur (Dullemond & Dominik 2005; Zsom et al. 2010). Grain growth in protoplanetary discs has been the subject of theoretical (Stepinski & Valageas 1997; Suttner & Yorke 2001; Dullemond & Dominik 2005; Haghighipour 2005; Ciesla 2007; Laibe et al. 2008; Ormel & Klahr 2010; Birnstiel et al. 2012), and experimental investigation (Blum et al. 2000; Blum & Wurm 2000, 2008; Teiser & Wurm 2009).

However, to date, there is no complete full 3D analysis of the dust dynamics (vertical settling and radial drift) of a chemically heterogeneous dust mixture. The aim of this work is, thus, to simultaneously investigate the effects of grain growth, size and density in shaping the dust distribution of a multicomponent dust mixture at large disc scales, and to gain more insight into the dynamical processes which may have contributed to assembling chondritic material and the building blocks of planets.

2 METHODS

We compute the vertical settling, radial drift and growth of a multicomponent dust using our 3D, two-fluid (gas+dust) SPH code (Barrière-Fouchet et al. 2005; Laibe et al. 2008). In this section we describe the structure of our chosen protoplanetary disc, section 2.1, the adopted grain chemistry, section 2.2, the prescription used for grain growth, section 2.3, and detail our simulations, section 2.4.

2.1 Disc Model

In order to make comparisons with previous work, we consider a typical T-Tauri disc used in Barrière-Fouchet et al. (2005) and Laibe et al. (2008) as our fiducial disc model, which represents the initial state of our simulations. The mass of the central star is \( M_\ast = 1 M_\odot \), and the disc is described by the following parameters: the mass of the disc is \( M_{\text{disc}} = 0.02 M_\ast \), with a radial extension of \( 20 \leq R(\text{au}) \leq 400 \). The disc is composed of 99% gas and 1% dust by mass. The parametrization for the temperature reads as \( T \propto R^{-3/4} \), and for the surface density as \( \Sigma \propto R^{-3/2} \). The disc is vertically isothermal and the sound speed is \( c_s \propto R^{-3/8} \). The vertical scale height is \( H = c_s/\Omega K \), and \( H/R \propto R^{1/8} \). The disc is flared and \( H/R = 0.05 \) at our reference radius, \( R_0 = 100 \text{ AU} \). For all simulations, the artificial viscosity is set to \( \alpha_{\text{crit}} = 0.1 \) and \( \beta_{\text{crit}} = 0.0 \), emulating a viscosity parameter \( \alpha_{\text{crit}} = 0.01 \) (Shakura & Sunyaev 1973; Fouchet et al. 2007), to reproduce the observed stellar accretion rate (King et al. 2007).

2.2 Grain Chemistry

Dust in discs is a complex mixture of several species. The chemistry of the dust is strictly related to the physical conditions in each zone of the disc and to the composition of the gas and the pristine dust (Gail 1998). In the hotter inner zone of the disc, dust experiences several chemical processes such as direct condensation from the gas phase, annealing, melting, shocks, and gas-grain surface interaction (Henning & Semenov 2013). In the cooler outer part of the disc, the low temperatures and slow kinetics prevent all these processes to occur efficiently and the majority of the dust will generally keep its pristine chemical composition and structure for longer time-scales. Our disc extends from \( 20 \leq R(\text{AU}) \leq 400 \), thus we do not take in account any chemical transformation of the dust grains. Furthermore, since the inner limit of our disc is beyond the major ice
The occurrence of ice lines could change the chemical composition of the dust, by removing or adding components, and alter the dust size distribution of grains. Nevertheless, the overall dynamical behaviour of grains will still be ruled by their resulting aerodynamic parameter, $\zeta$.

### 2.3 Grain Growth

Observations of pristine dust in protoplanetary discs are characterized by aggregates with sizes of the order of sub-microns to microns (Testi et al. 2014). In our simulations the initial grain size, $s_0$, is common for all particles, and is set to $10 \mu m$. Laibe et al. (2008) show that the results of their simulations with grain growth have little dependence on $s_0$ when the initial size is in the sub-micron to micron range.

Aggregates in discs are made of different pristine components, which we call grains. In section 2.2 we assumed that our initial grains comprise the species in Table 1 with their relative abundances (Pollack et al. 1994). Grain growth is a complex process, and as first order approximation one could assume that growth occurs as a result of random collision between components of the same or different species. The resulting aggregates would be characterized by a distribution of densities which ranges between the two extremes we consider here (iron and ice), with populations of iron-, silicate- and ice-enriched grains. Due to the initial abundance differences of our species, the resulting aggregates will maintain a spread in their densities, as it is unlikely to produce only one single final group of aggregates characterised by the same type of mixture.

Dynamics dictates how aggregates will evolve in a disc. Laibe et al. (2008) and Laibe (2014); Laibe et al. (2014a,b) investigated in detail the differences in the timescales between vertical settling and growth rates, and between radial drift and growth rates. They concluded that the vertical settling is almost one hundred times faster than the radial drift, and that these two dynamical events can be considered as separate. Moreover, grains grow moderately during the settling phase compared to their final size ($s = 100 \mu m$, at 100 (au), see appendix A) and the efficiency of growth increases once the grains settle in the midplane.

Since the initial size of our grains, $s_0$, is equal and common for all particles (10 $\mu m$), grains with different compositions will behave differently as their stopping time is a function of their density (see equation 1). Given the moderate growth of grains during vertical settling, the settling can result in inhomogeneities in the chemical content of the disc. In the midplane, the radial drift is then dictated by $\zeta$ (Weidenschilling 1977). Aggregates of the same size but different compositions will drift at different velocities. These considerations suggest that grain dynamics in the disc should, in fact, enhance chemical inhomogeneity. Evidences from meteorites also point to the presence in the Solar Nebula of different chemical reservoirs from which they accreted (Palme & Jones 2003; Scott & Krot 2005). The verification of these predictions and their evolution with time are some of the goals of this work.

Grain growth in our SPH code follows Laibe et al. (2008). Grains within an SPH dust particle are assumed to stick perfectly upon collision. Our prescription for grain growth is taken from Stepinski & Valageas (1997), where
Size and density sorting of dust grains in SPH simulations of protoplanetary discs

\[ \frac{ds}{dt} = \sqrt{\frac{2}{3} R_0 \alpha} \frac{\dot{\rho}}{\rho_i} \sqrt{\frac{S_c - 1}{S_c}}, \]

where \( R_0 \) is the Rossby number, \( \alpha \) the Shakura & Sunyaev (1973) turbulence parameter, \( \dot{\rho} \) the density of matter concentrated into solid particles, \( \rho_i \) the intrinsic density of the physical grains and \( S_c \) the Schmidt number.

In our simulations when aggregates grow they keep their intrinsic density constant, i.e. there is no mixed growth between particles of different species. This as a direct consequence of the growth prescription of Stepinski & Valageas (1997) which assumes collisions occur each time between two identical (size and density) spherical particles with growth occurring within a SPH particle (Laibe et al. 2008).

While it may appear non-physical to only consider growth between the same species, this simplified assumption does mimic the true density distribution of real growth between species of mixed composition. The initial difference in the abundances of components-grains and their dynamical dependence on density suggest that we will have, at any given time and location, aggregates with different compositions. Aggregates whose resulting density is iron-enriched will behave similarly to our “iron grains”, while aggregates which are characterized by a high ice content will behave similarly to our “ice grains”, and silicate-rich grains will behave similarly to our “pure silicates”. As such, having a fixed discrete distribution of \( \rho_i \) between two extremes (ice and iron) and four intermediate species will allow us to trace and investigate the different behaviours driven by the intrinsic density and the aerodynamic parameter. Any interpolation of the behaviour of aggregates with intermediate densities is then straightforward. In fact, this approach is similar to the widely used approximation to study the effect of size on dust dynamics for which a discrete grain size distribution and often one chemical species is considered (Barrière-Fouchet et al. 2005; Dullemond & Dominik 2008; Bai & Stone 2010; Charnoz & Tailliet 2012). These simulations proved to be in very good agreement with observations. Our simulations, instead, account for a discrete distribution of densities and a time-evolving distribution of size since we also include grain growth. Growth can erase the illustrated effect of densities only if, at any given time and location, grains with different composition reach the same value of \( \zeta \) before any of the dynamical forces (drift and settling) separate them. We demonstrate in appendix A, that this is never the case.

In our simulations, we do not consider dust fragmentation. Fragmentation occurs when the relative velocity of the particles becomes greater than the critical velocity (the velocity between colliding particles which will likely lead to a fragmentation of the dust rather than sticking) (Blum & Wurm 2008). The dynamics of growing and fragmenting dust of single composition have been studied in detail by Dullemond & Dominik (2005); Birnstiel et al. (2010, 2012); Gonzalez et al. (2015a) and more recently by Gonzalez et al. (2017). Dullemond & Dominik (2005) and Birnstiel et al. (2010, 2012) showed that a balance between growth and fragmentation can result in a steady distribution of different sizes in discs, especially in the inner disc zones. Gonzalez et al. (2017) found that growing and fragmenting grains can result in a self-induced dust trap.

The critical velocity is a function of the chemical composition and the porosity of the dust (Yamamoto et al. 2014). Preliminary tests for our disc model with the most recent theoretical values of 30-36 m s\(^{-1}\) derived from Yamamoto et al. (2014) for silicate aggregates made of monomers of 0.1 \( \mu \)m, show that this critical velocity is hardly reached in our large disc, and the effects of fragmentation are negligible within the considered evolutionary time. We assume that no changes in the critical velocities occur with time, size of grains (always considered as grains made of monomers of 0.1 \( \mu \)m), and species. However, critical velocities of different species, such as ice, silicates, iron and sulfides, are still uncertain (Wada et al. 2009; Teiser & Wurm 2009; Wada et al. 2013; Yamamoto et al. 2014) and they need to be assessed before implementation.

For this reason, we decided not to include fragmentation at this stage. Fragmentation of grains will be investigated in a future work.

2 Same as in Barrière-Fouchet et al. (2005) and Laibe et al. (2008) the gaseous disc is evolved for a given time to let the pressure and artificial viscosity smooth the initial velocity field and the shape of the gaseous disc. Moreover, particles which, at any given time, move out the disc boundaries are removed from the calculation.
inner disc with particles reaching cm-sizes in a few thousand years. Similarly to Laibe et al. (2008), our simulation shows that efficient growth is experienced by grains in the inner region and, as expected, we see that denser grains generally reach smaller sizes. This behaviour results directly from the prescription of growth derived by Stepinski & Valageas (1997), with \( ds/dt \propto c_s \rho_0^{-1} \).

One may wonder why grains having reached their optimal drift size are not lost to the star but stay in the inner disk where they continue to grow, and whether this is a numerical artefact. In their SPH simulations, Lodato & Rice (2004) found that the inner boundary conditions produced an outward erosion of the disc inner edge resulting in a gas pressure maximum slightly exterior to it, which would be capable of trapping drifting grains. However, the expectation that fast-drifting grains leave the disk before reaching large sizes comes from analytical (Weidenschilling 1977) and numerical (Brauer et al. 2008a; Birnstiel et al. 2010) work neglecting the drag back-reaction of dust on gas. On the contrary, several studies taking back-reaction into account (see e.g. Laibe et al. 2008; Fouchet et al. 2010; Gonzalez et al. 2015a; Drążkowska et al. 2016) have shown that it slows down the drift of grains and, combined with their faster growth closer to the star, results in a pile up in the inner disc. This is also what happens in the simulation presented in this paper (for a detailed discussion of the role of back-reaction, see Gonzalez et al. 2017).

In Laibe et al. (2008) the evolution of the radial size profile is driven by the rate of radial drift caused by the optimal drift size of one species, i.e. in our case, the evolution of the growth profile is not only driven by the size of the particles, but by the aerodynamic parameters \( \zeta = \rho_0 \) and by the optimal drift size proper to each species (see equations 3 and 4). The effects of grain growth on the evolution of the dust distribution will be discussed in detail in sections 3.3 and 4.

### 3.2 Vertical settling

Figure 5 shows the distribution of the icy (water ice plus organics), silicates, sulfides and iron particles respectively, at four evolutionary stages for the disc seen edge-on: a fast vertical settling is followed by a very efficient radial drift of denser particles. It is evident that the chemical characterization of the dust particles is driving the dynamics of the dust at different rates, e.g. icy particles settle toward the midplane, remixing with the silicate-iron-rich dust. This second stage of vertical settling can be explained by the evolution of the aerodynamic parameter for single species. In Fig. 7 the icy particles for which \( \zeta_{\text{icy}} \leq \zeta_{\text{sil}} \) are the particles which populate the icy contour of the disc in Fig. 5. As grain growth proceeds, \( \zeta \) of the lighter material on the surface of the disk increases and becomes comparable to the values which characterised the denser material at earlier stages. We have a superimposition of the \( \zeta \) values with \( \zeta_{\text{icy}} \sim \zeta_{\text{sil}} \) and the vertical settling of the lighter material becomes more efficient. This phase of settling is, thus, size-driven.

A second phase of vertical settling starts immediately in the inner disc and, at later times, in the outer disc: the icy particles settle toward the midplane, remixing with the silicate-iron-rich dust. This second stage of vertical settling can be explained by the evolution of the aerodynamic parameter for single species. In Fig. 7 the icy particles for which \( \zeta_{\text{icy}} < \zeta_{\text{sil}} \) are the particles which populate the icy contour of the disc in Fig. 5. As grain growth proceeds, \( \zeta \) of the lighter material on the surface of the disk increases and becomes comparable to the values which characterised the denser material at earlier stages. We have a superimposition of the \( \zeta \) values with \( \zeta_{\text{icy}} \sim \zeta_{\text{sil}} \) and the vertical settling of the lighter material becomes more efficient. This phase of settling is, thus, size-driven.

The introduction of lighter material into the midplane is more efficient in the inner zone of the disc (see Fig. 5). At the end of our simulation and in the inner \( \sim 80 \) au, all the icy particles are introduced in the denser midplane. In the outer part of the disc a vertical chemical sorting can still be noticed. This behaviour is due to the lower growth rate in the outer disc (see Fig. 4, and Laibe et al. (2008)), where smaller and lighter icy grains will remain coupled to the gas longer.

\[
\begin{align*}
\text{Eq. 6} \quad t_{\text{sett}} &= \frac{Z}{\mu_{\text{sett}}} = \frac{4}{3} \frac{\sigma}{m} \Omega_{\text{c}}^2, \\
\end{align*}
\]

where \( m \) is the mass of a spherical particle and \( \sigma \) its cross section. Given that \( (\sigma/m)\propto(\rho_0 \Omega)^{-1} = \zeta^{-1} \), equation 6 states that, for given conditions, \( (\rho_0 \Omega_0^2/\rho_1) \), and distance to cover, \( Z, \) larger-heavier particles will have smaller \( t_{\text{sett}} \) or will settle at higher speed than smaller-lighter particles. In this case, two grains made of different material, \( i \) and \( j \), but with the same size would have \( t_{\text{sett}}(i)/t_{\text{sett}}(j) \propto (\rho_i/\rho_j) \). As an example the \( t_{\text{sett}}(\text{ice})/t_{\text{sett}}(\text{iron}) = 8.55/7.87 = 4/3 \) times longer than \( t_{\text{sett}}(\text{iron}) \), and in order to erase the effect of density ice particles should grow 8.55 times larger than the iron particles before they separate. Figure 6 (middle) and Fig. 6 (bottom) show that during the first phase of vertical settling growth is not efficient to counterbalance the strong effect brought by the intrinsic density of grains (in the first couple of kyr of our simulation the \( s_{\text{ice}}/s_{\text{iron}} \) ratio is always in the order of 1-1.2). Thus, when the size of two particles is comparable, which is the case in the early evolution, the vertical settling is density-driven.
Size and density sorting of dust grains in SPH simulations of protoplanetary discs

3.3 Radial drift

After the first $\sim 40 - 50$ kyr, the radial drift of the dust starts to become extremely efficient for the denser grains (see Fig. 5). We see a radial sorting of chemical species with time. The outer disc becomes depleted in heavy particles in $\sim 50$ kyr. Figure 8 shows the surface density of different species at the end of the simulation: the disc outside $\sim 110$ au is iron-depleted, outside $\sim 200$ au sulfide-depleted and outside $250$ au silicate-depleted. The regions beyond $250$ au are ice-rich. The different maximum values of the surface densities are due to the differences in the initial amount which characterizes each species.

As reported in the introduction, the dust radial drift is driven by the optimal drift size proper to each dust particle (see equations. 3 and 4). In Fig. 4 we reported the evolution of the radial profile of $s_{\text{opt}}$ for water ice and iron at different evolutionary stages. Iron particles have a smaller optimal drift size than water ice particles. Looking at Fig. 4 it can be seen that the smaller optimal drift size for iron particle is leading to a radial chemical sorting of the dust. Similar to iron, sulfides and silicates follow the radial drift dictated by their $s_{\text{opt}}$. Not all the water-ice particles in the outer disc reach their optimal drift size by the end of the simulation, making the radial drift of ice overall less efficient.

Figure 9 tracks the radial drift (top), $s/s_{\text{opt}}$ (middle), with $s_{\text{opt}}$ calculated using equation 3, and the size (bottom) as a function of time for three particles with different intrinsic density (water-ice, silicate and iron) which are located at the same position at the beginning of the simulation. As the growth proceeds, the iron particle reaches the $s/s_{\text{opt}} = 1$ point before the lighter particles and starts to drift inward more efficiently. Lighter particles keep growing in place before reaching their optimal size and starting to drift toward the inner regions of the disc.
4 DISCUSSION

Our results are in good agreement with those found by Laibe et al. (2008), Laibe (2014), Laibe et al. (2014a), and Laibe et al. (2014b), who studied the dynamics of growing but not fragmenting grains illustrated in section 2.3. Furthermore, we confirm that, (i) a very efficient vertical chemical sorting of the dust starts at the beginning of the simulation, and (ii) the density driven vertical settling which produces the initial chemical sorting is the first dynamical mechanism expected when the size of the grains is comparable. Moreover, the grain growth within our disc model is not efficient enough to counterbalance this process.

Our results show that, as the intrinsic density of the growing grains determines the optimal drift size, the radial drift of different species would produce a radial chemical sorting of the dust. As a consequence of the vertical settling and radial drift, the disc will lose its initial chemical homogeneity, with inhomogeneities occurring from the beginning of the simulation. These results could bring dramatic consequences in the composition of the building block of meteorites parent bodies and planetesimals. The chemical and dynamical evolution of the dust in our disc is thus the main focus of this section. We will discuss the physical properties of the particles in section 4.1 and the evolution of the chemical content in our disc in section 4.2.

4.1 Size and density sorting

Using our set of diagnostic we are able to trace all the properties of every SPH particle at any given time. At the end of the simulation, we randomly sampled groups of water ice and silicates particles which are located at the same coordinates in the midplane and record their size and intrinsic density. We replicate this measurement at different radial distances from the central star. We chose ice and silicates particles as they are still present at large radial distance at the end of the simulation. In Fig. 10 we thus plot the average size of water-ice particles versus the average size of silicate particles at different radial distances from the star (colours). The brown line represents the theoretical size of water-ice...
time evolution of $s$ for the points laying at $R<100$ au, $Z<9$ au) at the beginning of the simulation. Middle: time evolution of $s_{\text{ice}}/s_{\text{sil}}$ (red) and $s_{\text{ice}}/s_{\text{iron}}$ (blue) ratio. Bottom: size as a function of time for the three different particles. At the beginning of the simulation when the size of the particles is comparable, the vertical settling is density driven and will lead to a vertical chemical separation according to the intrinsic density of the grains. The curve of the $s_i/s_j$ ratios reaches a peak after 11 kyr and then decrease: ice particles grow bigger, thus the ratio increases. When the silicates and iron particles settle toward the midplane, they grow faster than ice, as they are in a denser environment and thus the $s_i/s_j$ ratios starts to decrease. However, after a few thousand years we are already tracing particles which are far from each other and, thus, experiencing different local conditions.

Particles predicted by the following equation

\[ s_{\text{ice}} = s_{\text{sil}} \frac{\rho_{\text{sil}}}{\rho_{\text{ice}}}, \]

i.e. the predicted size of water-ice particles if perfect size-density sorting with silicates particles occurs ($\zeta_{\text{ice}} = \zeta_{\text{sil}} = (s\rho)_{\text{ice}} = (s\rho)_{\text{sil}}$).

The returned correlation coefficient between the average size of silicates and average size of the ice particles for all the data points within $R<100$ au in Fig. 10 is $R_c=0.99$, while for the points laying at $R \geq 100$ AU the correlation coefficient is $R_c=0.64$. The inner midplane of the disc is generally aerodynamically (size-density) sorted. This is less evident in the outer part of the disc, where the lower growth rate and the lower gas density causes the aerodynamic sorting to occur more slowly. Thus, in case of pure growth particles tend to naturally sort in the disc according to their aerodynamic parameter.

Our finding confirms that aerodynamic sorting can be an active mechanism which characterizes the disc at very large scales and suggest that the sorting trend observed in chondrites could thus have occurred not only in a local environment but also at disc scales. Since the aerodynamic sorting in chondrites could have occurred between chondrules and metal-troilite grains within the same chondrite group (Benoit et al. 1998; Friedrich et al. 2015), we investigate the aerodynamic sorting between different species in more detail in section 4.2.1.

4.2 Disc chemical and dynamical evolution

As discussed in section 3, vertical settling and radial migration continuously change the distribution of dust particles in different regions of the disc.

In order to quantify in more details the change in the chemistry in the whole time range, we report in Fig. 11, from left to right, the evolution of the dust mass content (normalized to the mass present at the beginning of the simulation), the evolution of the $H_2O/\text{Si}$ and $\text{Fe}/\text{Si}$ ratios (all values normalized to our “solar” values in Table 1), in the disc midplane ($-1 < Z(\text{au}) < 1$) (top row), and in the disc surface where $|Z(\text{au})| > 1$ (bottom row). The selected disc radial extension is $20 < R(\text{au}) < 100$.

The $H_2O/\text{Si}$ and $\text{Fe}/\text{Si}$ ratios at the surface of the disc are plotted until the dust mass, $m_{\text{d}}$, drops to 10% of the initial mass. Close to this value the ratios are biased by the small number of particles present. The time resolution of all the plots is $\Delta t \sim 159$ yr. This allows to investigate the variation with time of the chemical content in our disc in very good detail, as this value represents 1/1000 of the total time of the simulation. Moreover, these plots will give us an idea of the chemical composition of the dust from which aggregates could accrete at a given time.

Looking at Fig. 11, the effects of the dynamics on the chemical distribution of the dust become clearer. For the $H_2O/\text{Si}$ ratio, in the midplane, we see (1) the enhancement of iron due to the density-driven settling; (2) the size-driven vertical settling then increases the amount of ice which is populating the midplane. When the dust radial drift starts to become more efficient, (3) we see that silicate particles from the outer disc are populating the inner disc midplane, thus decreasing the $H_2O/\text{Si}$ ratio. At later stages, (4) the radial drift of the ice increases the $H_2O/\text{Si}$ ratio. On the other hand, for the $\text{Fe}/\text{Si}$ ratio, we see (1) the enhancement of iron due to the density-driven

\[ \text{Fe}/\text{Si} = (\frac{\rho_{\text{iron}}}{\rho_{\text{sil}}}). \]

All values are then normalized to the “solar” values in Table 1.
vertical settling; (2) the amount of silicate particles is then increased by the size-driven vertical settling. When the dust radial drift starts to become more efficient (3) iron particles populate the inner disc midplane, and, at later stages, (4) the radial drift of the silicates decreases the Fe/Si ratio.

At the same time, on the surface of the disc, the dust content is reduced in heavier compounds. The H$_2$O/Si ratio increases due to the vertical settling of the silicate particles. The trend does not change with time as the vertical settling of the icy particles does not become so efficient to invert and lower the H$_2$O/Si ratio within the time ($t \sim 20$ kyr) for which we reach the cut-off (the mass of the particles present in the selected zone reaches 10% of the initial mass). The Fe/Si ratio becomes “sub-solar” due to the vertical settling of the iron particles, until the density-driven phase is replaced by the size-driven phase when silicate particles also start to settle more efficiently due to their growth. As a consequence the Fe/Si ratio starts to move again towards higher values.

Similarly to Fig. 11, in Fig. 12 we report the dust mass ratio and the chemical ratios in the disc midplane (top) and surface (bottom) for 100 < $R$(au) < 200. We see a different behaviour of the mass of particles which populate the disc midplane at different times: (a) the amount of dust in the midplane increases due to the dust vertical settling, and (b) at $t \sim 50$ kyr due to the radial drift of the dust coming from the outer regions of the disc. The behaviour of the chemical ratios at these early stages is similar to that found in Fig. 11. However, at $t \sim 80$ kyr we see (c), a steep decrease of the dust mass of the disc and, at the same time, a decrease of the Fe/Si ratio. At $t \sim 120$ kyr, (d), a second fast depletion of dust occurs and the H$_2$O/Si increases. This behaviour can be explained by the radial drift of the iron particles which starts as soon as their optimal drift size is reached (c), and

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**Figure 7.** Aerodynamic parameter for icy (black) grains and silicates (red) grains at four evolutionary stages. The double tail for the icy grains is caused by the fact that we are considering all the three icy populations (water ice, volatile organics and refractory organic) which have intrinsic density $0.92 \leq \rho_1 \leq 1.5$. When the size of the grains with different density is comparable, the heavier grains separate from the lighter grains and start to settle toward the midplane. As the lighter grains grow, their aerodynamic parameter increases and they start to behave as heavier grains and settle toward the midplane. After $t \sim 50$ kyr, the vertical chemical separation of grains in the inner disc out to 80 AU is lost.
Figure 8. Surface density of water-ice, silicates, sulfides and iron particles at the end of the simulation. The chemical radial sorting is evident. The differences in the values of the surface densities are due to the different initial amount which characterizes each species.

Figure 9. Top: radial drift for water ice, silicates and iron particles as a function of time. \(s/s_{opt}\) (middle) and \(s\) (bottom) as a function of time for the same particles. Denser particles have smaller optimal drift size. As particles grow, iron particles reach their optimal drift size before lighter particles and thus, start to drift inward before the lighter particles.

Figure 10. Average size of silicates versus average size of ice particles at different distances from the protostar (color). The brown line represents the theoretical size of ice grains predicted using equation. The dust in the inner disc \((R < 100 \text{ au})\) is aerodynamically sorted with a correlation coefficient of 0.99. This sorting is less evident beyond 100 au, where the predicted trend is not fully satisfied with a correlation coefficient of 0.64.

On the disc surface the chemical ratios are characterized by the similar behaviour found in Fig. 11 for the early evolutionary stage: in this part of the disc surface, the Fe/Si ratio drops to “sub-solar” values (density-driven settling) before returning to “super-solar” values (size-driven settling). The \(H_2O/Si\) ratio increases because of the density driven vertical settling of the silicates, then decreases because of the size driven vertical settling of the ice particles.

The second drop in the Fe/Si ratio which starts at \(t \sim 60–80 \text{ kyr}\), is then due to the radial drift of the iron which at this stage is more efficient than the silicates one, and the \(H_2O/Si\) ratio increases because of the radial drift of the silicates which is more efficient than the ice one. However, at this stage, the total mass in this region already dropped under 20% of the initial value and the results start to get biased by the small number of particles.

In conclusion, when we look in this disc zone, we are also observing the transit of the denser dust which is leaving the outer regions of the disc and crossing this zone to populate the inner disc.

4.2.1 Analogies with chondrites

In the previous sections we showed that at early stages, when the size of the pristine dust is comparable, the density-driven vertical settling will separate the denser particles from the lighter particles leading to dust chemical sorting. Our results also show that chemical sorting can also occur via radial
drift: the resulting inner disc is enriched with denser material while the outer disc is characterized by a high ice content. We also showed that the combined effects of vertical settling and radial drift continuously change the chemical content of the disc.

Physical sorting and grain segregation are thought to be possible mechanisms which produced dust fractionation in pristine grains in the Solar nebula and the metal-silicate fractionation observed in meteorites (Kuebler et al. 1999; Zanda et al. 2006). This sorting may have been one of the mechanisms which produced the different chemical compositions among the different clans of chondrites and the differences found among chondrites groups belonging to the same clan (Palme & Jones 2003; Wood 2005; Scott & Krot 2005).

However, there is still a debate about the efficiency of aerodynamic sorting and on the location at which dust chemical sorting might have occurred. It has been suggested that different evolutionary times and radial distances from the forming Sun had played a major role in determining the physical and chemical sorting of dust in the Solar nebula.
final structure of the chondrites parent bodies (Scott & Krot 2005).

In our simulation we are considering a large disc, thus we cannot directly compare our results with the chemical and dynamical evolution of the chondrites which formed in the inner Solar Nebula. However, an indirect comparison within the frame of our disc may help to find some analogies and determine if, when and where aggregates in our disc model can resemble the major properties of chondrites, and thus, suggest pathways of formation for these objects.

In the following discussion we consider silicate and iron particles in our disc respectively as the possible chondrules precursors (or already formed chondrules) and the metallic grains in chondrites. The mechanism (or mechanisms) from which chondrules originated is still not well constrained (shock waves, planetesimals impacts, lightning, jets, winds (Scott & Krot 2005)), and more recent analysis suggests that chondrules formation may have started contemporaneously with CAIs (the oldest objects in our solar system) in a condensation process which lasted $\sim 3$ Myr (Connelly et al. 2012). As such it is not unreasonable to consider the presence of a sparse population of chondrules in the disc since the early stages of the protoplanetary disc evolution.

Our results show that radial chemical sorting characterizes the disc only when large scales are taken into consideration. The Fe/Si ratio in our inner midplane $20 < R(au) < 100$ is always barely “super-solar” with a deviation close to 1% (see Fig. 11), while the Fe/Si of chondrules moves from solar (ordinary chondrites) toward sub-solar values (Righter et al. 2006) (see Fig. 2). Thus, aggregation of “sub-solar” material in this location can be excluded.

We found that the Fe/Si in the midplane where $100 < R(au) < 200$ (Fig. 12) is “super-solar” until later stages (t~80 kyr) when the fast radial drift starts to deplete the denser dust in this region. In this case assembling dust in this part of the midplane might lead to chemically fractionated aggregates, with “sub-solar” Fe/Si ratios.

However, in order to produce fractionation in the outer midplane, time scales in the order of 60 kyr are needed to lower the Fe/Si ratio from 1 to 0.9 (see Fig. 12). This is in case of a clean and efficient radial drift. Indeed, the radial drift of dust, and thus, the chemical sorting, can be slowed down and/or stopped by the presence of particle traps in the disc. Particle traps are thought to be locations at which a fast and efficient pile-up and growth of dust occurs, making the formation of larger planetesimals more favourable.

Particle traps can occur from the early stages of the protoplanetary disc evolution inside vortices (Barge & Sommeria 1995; Johansen et al. 2004), at the ice-lines and at the edge of the dead zone (Kretke & Lin 2007; Brauer et al. 2008b), in discontinuities of the gas distribution in discs (Pinilla et al. 2012) or in self-induced dust traps (Gonzalez et al. 2015b, 2017). Particle traps can, thus, slow down or totally stop the radial chemical separation of the dust.

Vertical settling produces instead dust fractionation all along the disc surface (see Figs. 11 and 12). The disc surface is the only region in which we find “sub-solar” values of Fe/Si ratio from the beginning of our simulation. Aggregates in the surface of the disc can have “solar” values of the Fe/Si ratio at the beginning of the simulation, and “sub-solar” values a few thousand years later.

Furthermore, grain growth experienced by particles, and described in section 3.1, suggests that aggregates with different Fe/Si ratios could also contain grains with different sizes. In Fig. 13 we superimpose, on the left column, the Fe/Si ratio and the average diameter of silicate and iron particles as a function of time, for the disc surface ($|Z(au)| > 1$) where $20 < R(au) < 100$ (top), where $100 < R(au) < 200$ (middle), and for the disc midplane ($-1 < Z(au) < 1$) where $100 < R(au) < 200$ (bottom). In the right column we trace the ratio between the aerodynamic parameters of iron and silicate particles, $\zeta_{iron}/\zeta_{sil}$, as a function of time. The aerodynamic parameters are calculated using the average size of silicate and iron particles multiplied by their respective intrinsic densities. The closer the value of $\zeta_{iron}/\zeta_{sil}$ is to 1, the closer to a perfect size-density sorting the particles are. Thus, Fig. 13 allows to simultaneously check the chemical fractionation of the dust, the average grains diameter, and the aerodynamical sorting of grains in three different zones of the disc and at each time step of our simulation.

We see that aggregates with lower Fe/Si ratio will also have bigger grains. Furthermore, Fig. 13 (right column) shows that as soon as the simulation starts, the $\zeta_{iron}/\zeta_{sil}$ ratios move quickly towards values indicating a good degree of size-density sorting.

In the disc surface where $20 < R(au) < 100$, values of Fe/Si < 1 are associated with grains diameter in the order of 0.1–1 mm and a $\zeta_{iron}/\zeta_{sil}$ value which can reach $\sim 1.2–1.1$ over timescales ranging between 8 and 18 kyr. In the disc surface where $100 < R(au) < 200$ we see a Fe/Si < 1 ratio for the first 30 kyr, with grains having an average diameter in the order of 0.1 to 1 mm and with $\zeta_{iron}/\zeta_{sil}$ which can reach $\sim 1.1$. At $t \sim 70$ kyr, the Fe/Si ratio drops a second time under 1, the grain diameter is in the order of mm and the $\zeta_{iron}/\zeta_{sil}$ ratio moves toward higher values. At this evolutionary stage, the total dust mass already dropped under 20% of the initial amount (see Fig. 12), and thus, we are starting to sample the residual dust on the disc surface which did not grow/sort efficiently.

In the midplane where $100 < R(au) < 200$, after $t \sim 80$ kyr, when the Fe/Si ratio moves to subolar values, the $\zeta_{iron}/\zeta_{sil}$ moves away from a perfect size-density sorting. However, the values of the $\zeta_{iron}/\zeta_{sil}$ ratios, when $80 < t(kyr) < 140$, are still compatible with a good degree of aerodynamical sorting (1 $\leq \zeta_{iron}/\zeta_{sil} < 1.2$). Here, the average diameter of the iron and silicate particles when the Fe/Si starts to become “sub-solar” is in the order of mm to cm (see Fig. 13 bottom). Aggregates in this region would have bigger grains (mm to cm), experience chemical fractionation and a general aerodynamical sorting. Then, as already shown in Fig. 10, at the end of the simulation, the residual aggregates in the outer discs will be less aerodynamically sorted although fractionation in their Fe/Si persists.

For completeness, we report in Fig. 14 the Fe/Si ratio, the average diameter of iron and silicate particles and the $\zeta_{iron}/\zeta_{sil}$ ratio for the inner midplane where $20 < R(au) < 100$. It can be seen that particles in this zone of the disc move toward a perfect size-density sorting. The sorting in this zone is achieved almost immediately, just after the beginning of the simulation.

We thus find a trend which is compatible with a fractionation of the Fe/Si ratio and the size of the chondrules and iron grains found in different groups of chondrites. However, the values of the Fe/Si ratios returned by our simula-
Figure 13. Left column: Fe/Si ratio (black) and average diameter of iron and silicate particles (blue) as a function of time. Top: disc surface \((|Z(\text{au})| > 1)\) where \(20 < R(\text{au}) < 100\). Middle: disc surface where \(100 < R(\text{au}) < 200\). Bottom: disc midplane \((-1 < Z(\text{au}) < 1)\) where \(100 < R(\text{au}) < 200\). Right column: \(\zeta_{\text{iron}}/\zeta_{\text{sil}}\) for the three selected zones, calculated multiplying the average size of iron and silicates with their respective intrinsic densities. A perfect size-density sorting would occur when these ratios are equal to 1. The \(\zeta_{\text{iron}}/\zeta_{\text{sil}}\) ratios decrease quickly towards 1 suggesting that the system evolves towards size-density sorting. However, in the outer surface, after 70 kyr, and in the midplane, after 80 kyr, when the Fe/Si ratio moves to “sub-solar” values, the \(\zeta_{\text{iron}}/\zeta_{\text{sil}}\) moves away from a perfect size-density sorting.
Size and density sorting of dust grains in SPH simulations of protoplanetary discs

15

Figure 14. Left column: Fe/Si ratio (black) and average diameter of iron and silicate particles (blue) as a function of time for the disc midplane (−1 < Z(au) < 1) where 20 < R(au) < 100. Right column: $\zeta_{iron}/\zeta_{sil}$ for the selected zone, calculated multiplying the average size of iron and silicates with their respective intrinsic densities. A perfect size-density sorting would occur when these ratios are equal to 1. The $\zeta_{iron}/\zeta_{sil}$ ratio move quickly towards 1 suggesting that in this zone of the disc, grains move towards a perfect sorting within few years after the beginning of the simulation.

Ratios are not low enough when compared with the observed Fe/Si ratios in chondrites (Righter et al. 2006). This is because of our adopted spatial resolution. When calculating our ratios in the disc surface, we are considering, for a given interval in $R$, all the vertical extension of the disc for which $(|Z(au)| > 1)$, thus losing resolution in $Z$.

Figure 5 shows that there are zones in the disc surface for which the Fe/Si ratios can reach very low values, and 0 where iron particles are not present. Thus, as an example, we report in Fig. 15 the Fe/Si and the $\zeta_{iron}/\zeta_{sil}$ ratios for the disc surface where $|Z(au)| > 5$ and $20 < R(au) < 100$. Ratios are plotted until the number of iron particles reaches 0. It can be seen that, when a different vertical section of the disc is considered, the Fe/Si ratios can reach very low values, more compatible with the observed trend in chondrites, although, in this case, the size-density sorting is less efficient with a $\zeta_{iron}/\zeta_{sil}$ moving toward a minimum value of $\sim 1.4$.

Furthermore, as already pointed out, chondrites did not form at this very large disc scales, but in the inner few au of our Solar nebula. This suggest that a similar process might have also occurred in the inner disc, with different time-scales or with different efficiency.

A simple extrapolation of our results would imply that the aggregation of chondritic material could have occurred in the surface of the inner young Solar Nebula during the two phases of vertical settling where size-density sorting was also efficient. The differences found among chondrites clans might then be ascribed to the different radial distance at which this process occurred. This distance could have then determined, for example, the amount of water accreted from the chondrite parent bodies. Indeed accretion of E chondrites likely occurred in the inner warmer region of the disc within the snow-line, ordinary chondrites close to the snow-line and carbonaceous chondrites beyond the snow-line (Scott & Krot 2005; Wood 2005).

These results only represent a starting point in the study of the dynamics of chondrites. Indeed, more complex models are needed to explain not only the variations in the Fe/Si ratios but also among other elements.

In our next study we will explore the growth and the aerodynamic sorting of a multicomponent dust in the inner disc accounting also for dust fragmentation.

4.3 Analogies with discs observations

In the previous sections we showed that grains decouple from the gas and settle toward the midplane according to their density and size. Moreover, as grains reach their optimal drift size, they start to drift toward the inner region of the disc.

In Fig. 16(top) we plot the grain size distribution at $t = 42970$ yr, as a function of $R$ and $Z$. This timestep is the same as the top-right panel in Fig. 5 where we plotted $\rho_d$ as a function of $R$ and $Z$. That figure is reproduced in Fig. 16(bottom) for ease of comparison.

In terms of size, our results are in good agreement with previous simulations made by Barrière-Fouchet et al. (2005) who studied the dust distribution of grains with different size and found that larger grains pile up in the disc midplane while smaller grains distribute in the disc envelope. We are also in agreement with the sorting trend observed in GG Tau and TW Hya described in section 1.

Looking at the evolution of the chemical distribution in Fig. 5 and comparing it with the size distribution in Fig. 16 a qualitative observable prediction of the chemistry and physical properties of the dusty grains would read as smaller, lighter grains at the discs surface. This is in agreement with the dust properties of protoplanetary derived by infrared ob-
Figure 15. Left column: Fe/Si ratio (black) and average diameter of iron and silicate particles (blue) as a function of time for the disc surface (|Z(au)| > 5) where 20 < R(au) < 100. Right column: \( \zeta_{\text{iron}}/\zeta_{\text{sil}} \) for the selected zone.

servation (Bouwman et al. 2008; Meeus et al. 2009) where micron-size silicates particles are used to fit the infra-red spectra of the surface of the dusty discs around young stellar objects.

Moreover our results can help to disentangle the chemical dust composition of the disc within the midplane, which cannot be probed by observations (Williams & Cieza 2011). We suggest that the inner disc midplane could be enriched in denser material, iron and silicate-rich aggregates, while the outer disc regions would host ice-rich and iron-poor materials (see Fig.8). This prediction is also consistent with the chemical radial gradient generally found in the solar system when moving toward larger distances from the Sun (Lewis 2004): denser rocky planets in the inner regions while volatile-ice enriched bodies in the outer solar system.

Furthermore, our results suggest that planetary embryos might accrete from inhomogeneous material since the beginning of their formation with the location (radius) of their accretion determining their initial bulk elemental ratios.

5 CONCLUSIONS

We presented SPH simulations of grain growth and sorting of multicomponent dust in a protoplanetary disc using a 3D, two-fluid (gas+dust) SPH code.

We found that the dust vertical settling is characterized by two phases: the first phase is driven by the dust density which leads to a vertical chemical sorting of the dust; the second phase is size-driven which allows the enhancement of the concentration of lighter material in the layers deep inside the disc. We also see an efficient radial chemical sorting of the dust, with denser material rapidly drift in the inner zone of the disc. This process is driven by the different optimal drift size proper to each dust species.

Particles in the disc are aerodynamically (size and density) sorted in the inner regions, while in the outer regions the lower growth rates and the lower gas density prevent this sorting to occur efficiently. Particles move toward size-density sorting in very short time-scales. Our results are compatible with the observed large scale dust sorting observed in protoplanetary discs.

We see that the growth and dynamics of a multicomponent dust clearly produce chemical fractionation and aerodynamic sorting in large disc scales. It is interesting to note that large discs (20 \( \leq \) R (au) \( \leq \) 400) could produce, in a very short time (for example, t\(~\)5-20 kyr, in the inner disc surface), aggregates which would mimic the basic properties of chondrites. This suggest that dynamical chemical fractionation and aerodynamical sorting might have played an important role in determining their final aspect and chemical composition.

Moreover, our results open a new interesting question on the existence of undifferentiated and chemically fractionated aggregates which might have formed in the outer Solar Nebula during the early stages of the formation of our Solar System. We also suggest that planetary embryos might be characterized by inhomogeneous composition since the beginning of their formation.

6 ACKNOWLEDGMENTS

The authors are grateful to the LABEX Lyon Institute of Origins (ANR-10-LABX-0066) of the Université de Lyon for its financial support within the program "Investissements d’Avenir" (ANR-11-IDEX-0007) of the French government operated by the National Research Agency (ANR). We also acknowledge funding from PALSE (Programme Avenir Lyon Saint-Etienne). The authors wish to thank Sarah Maddison for helpful discussions and the anonymous referees for their useful comments which made us investigate in more detail our assumptions and the timescales of dynamics and growth, which improved the manuscript. All simulation were performed at the Common Computing Facility of LABEX LIO.
Figure 16. Top: Grain size distribution as a function of R and Z at \( t = 42970 \) yr. Bottom: Distribution of different chemical species as a function of R and Z. This figure reproduces the top-right panel in Fig. 5, for ease of comparison. Larger/heavier grains are located in the inner disc midplane while smaller/lighter grains are distributed in a wider zone. This in general agreement with observations.

APPENDIX A: DENSITY VERSUS GROWTH

In this appendix we investigate the efficiency of grain growth, vertical settling and radial drift. Our aim is to confirm that growth is not efficient enough to erase the inhomogeneity that different grain densities bring in the disc since the beginning of our simulations.

If grains with initially comparable sizes and different densities are located at the same position, in order to counterbalance the dynamical differences driven by densities, lighter grains should reach the same aerodynamic parameter, \( \zeta \), as denser grains before the vertical settling and/or the radial drift separate them.

Using our disc model in its initial configuration, we first solve equation 5 with a simple numerical integration (see Laibe et al. 2008) for three different grains with the same \( s_0 = 10 \, \mu m \) and different \( \rho_d \) (ice, silicates, and iron, with \( \rho_d \) taken from table 1). We assume that grains are located and locked in the same position. The chosen location is at \( R=100 \) au, our reference radius, and \( Z = H(R) \). We compute the time evolution of \( \zeta \) and estimate the time, \( t_\zeta \), at which grains reach the same value of the aerodynamic parameter. The gas density at \( Z = H(R) \) is calculated using

\[
\rho_g(Z) = \frac{\Sigma}{\sqrt{2\pi H}} \exp\left(-\frac{Z}{2H}\right),
\]

in Laibe et al. (2012). Then, we repeat the calculation in the midplane at \( R = 100 \) au. From Fig. 6 it can be seen that, once the particles reach the midplane, they have grown to sizes of the order of 100 \( \mu m \). We thus use \( s_0 = 100 \, \mu m \) as our reference size for this calculation.

Figure A1 shows the time evolution of \( \zeta \) for the three different particles calculated at \( R = 100 \) au at the disc surface (\( Z = H(R) \)) for \( s_0 = 10 \, \mu m \) (top) and in the midplane for \( s_0 = 100 \, \mu m \) (bottom). Note the change of scales for \( \zeta \). The timescales, \( t_\zeta \), for which three particles reach a similar value of \( \zeta \) is of the order of \( t_\zeta \approx 1000 \) yr.

We now calculate the initial velocity of settling, \( v_{set} \), and drift, \( v_{drift} \), proper to each grain. These quantities, multiplied by an interval of time, \( t \), give us an estimate of the separation which would occur between grains if they were allowed to move. We set \( t=1 \) yr, a value much smaller than \( t_\zeta \). If the resulting separation between grains is not negligible we can conclude that growth cannot counterbalance the inhomogeneities that densities are bringing into the disc.
Table A1. Radial separation at $R = 100$ au and $Z = 0$, between 100 $\mu$m size iron, silicate and ice particles (red) and vertical separation at $R = 100$ au and $Z = H(R)$, between 10 $\mu$m size iron, silicate and ice particles (black). Quantities are calculated after $t = 1$ yr and distances are expressed in km.

|     | iron | silicate | ice  |
|-----|------|---------|------|
| iron| 229  | 360     |      |
| silicate| 16790 |         | 132  |
| ice | 26460| 9670    |      |

In our calculations, $v_{\text{set}}$ is equal to

$$v_{\text{set}} = -\frac{\Omega^2 Z}{\rho_{\text{loc}} c_s} \zeta,$$

derived from equation 6, which is valid for small grain sizes (Dullemond & Dominik 2004).

$v_{\text{drift}}$ is calculated using the following equation from Brauer et al. (2008a):

$$v_{\text{drift}} = v_{\text{dust}} + \frac{v_{\text{gas}}}{1 + (St)^2}.$$

$v_{\text{dust}}$ is given by

$$v_{\text{dust}} = -2\nu \frac{1}{St + (1/St)},$$

where

$$\nu = \frac{c^2}{2V} \left( \frac{7}{4} + p \right).$$

$v_{\text{gas}}$ is equal to

$$v_{\text{gas}} = -3\alpha \frac{c^2}{V} \left( \frac{3}{2} - p \right),$$

where

$$V = \Omega R.$$
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