Chemical Evolution in a Protoplanetary Disk within Planet Carved Gaps and Dust Rings

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Abstract

Recent surveys of protoplanetary disks show that substructure in dust thermal continuum emission maps is common in protoplanetary disks. These substructures, most prominently rings and gaps, shape and change the chemical and physical conditions of the disk, along with the dust size distributions. In this work, we use a thermochemical code to focus on the chemical evolution that is occurring within the gas-depleted gap and the dust-rich ring often observed behind it. The compositions of these spatial locations are of great import, as the gas and ice-coated grains will end up being part of the atmospheres of gas giants and/or the seeds of rocky planets. Our models show that the dust temperature at the midplane of the gap increases, enough to produce local sublimation of key volatiles and pushing the molecular layer closer to the midplane, while it decreases in the dust-rich ring, causing a higher volatile deposition onto the dust grain surfaces. Further, the ring itself presents a freeze-out trap for volatiles in local flows powered by forming planets, becoming a site of localized volatile enhancement. Within the gas-depleted gap, the line emission depends on several different parameters, such as the depth of the gap in surface density, the location of the dust substructure, and the abundance of common gas tracers, such as CO. In order to break this uncertainty between abundance and surface density, other methods, such as disk kinematics, become necessary to constrain the disk structure and its chemical evolution.

Unified Astronomy Thesaurus concepts: Astrochemistry (75); Protoplanetary disks (1300); Planetary system formation (1257); Astronomical simulations (1857)

1. Introduction

Planets are born within young disks that formed from the collapse of a centrally concentrated dense core within molecular clouds. It is during the gas-rich protoplanetary disk stage that gas giant planets capture the volatile-rich gaseous material that will be part of their atmospheres. Therefore, giant planets have to be formed before the gas dissipates, a process that takes a few megayears (Alexander et al. 2014). Further, the physical state of protoplanetary disks is constantly evolving (Armitage 2011; Williams & Cieza 2011; Andrews 2020), and these changes can affect how planets form. For example, the initial composition and elemental budget of a planet would be different depending on the time and location of formation (Öberg et al. 2011; Cridland et al. 2016; Alessi et al. 2017).

Recent ALMA surveys of protoplanetary disks have shown that disk substructures are ubiquitous in protoplanetary disks, particularly axisymmetric ones (Zhang et al. 2016; Andrews et al. 2018; Long et al. 2018; Huang et al. 2018; Zhang et al. 2018). Among these axisymmetric substructures, the most common features are gas-depleted gaps and dust-rich rings. Within that context, it becomes important to constrain the chemical evolution during the early stages of planet formation. Previous works have explored the chemical changes taking place during disk evolution. Just to give a few examples: Eistrup et al. (2016, 2018) consider different initial abundances and the chemical evolution of the midplane including planet accretion; Facchini et al. (2017), Booth et al. (2017), and Krijt et al. (2018) take into account dust evolution. Clevees et al. (2013) explore the question of cosmic-ray ionization in protoplanetary disks, while significant emphasis has been placed on the evolution of CO abundance (Reboussin et al. 2015; Yu et al. 2017; Schwarz et al. 2018, 2019; Bosman et al. 2018). More recently, Facchini et al. (2018) post-processed hydrodynamic simulations within a thermochemical model, making predictions of line emission inside planetary gaps, and van der Marel et al. (2018) looked at the observable effects that different gap-carving processes have. Overall, the consensus is clear: gaps and rings will set the local conditions around forming planets.

There are several possible mechanisms to explain substructure formation. The primary theory is that young planets carve gaps in the dust and gas (Lin & Papaloizou 1986), inducing pressure bumps within the edges of the gaps (Armitage 2010; Pinilla et al. 2012, 2015; Zhang et al. 2018). The outer pressure bump then serves as a location where drifting dust will pile up, potentially evolve, and be observed as a ring (Dullemond et al. 2018; Andrews et al. 2018). However, there are other possible scenarios that produce pressure bumps. One of those scenarios takes place in the outer edge of the MRI dead zone in MHD simulations (Flock et al. 2015); another one occurs in the discontinuities produced by ice lines of abundant molecules, inducing dust growth (Zhang et al. 2016; Pinilla et al. 2017). Both gaps and rings are explained by the same mechanisms and are ubiquitous in protoplanetary disks.

The gap–ring substructure changes the local dust surface density and, consequently, the dust opacity. Depending on the location of the gap–ring substructure, variations in the dust surface density could change the chemistry in major ways (Cridland et al. 2017). Figure 1 is a sketch of the
phenomenology we expect to take place inside the gap—ring substructure. For example, there is a pileup of dust grains in the ring, and the gap gets hotter closer to the midplane because of its lower optical depth. Further, the propagation of high-energy photons, both far-UV (FUV) and X-rays, is enhanced, altering the local chemical equilibrium (Walsh et al. 2012). The high-energy photons photodissociate gas-phase species or photodesorb icy grain mantles, potentially fostering unique chemical signatures that would not otherwise be present (Cecchi-Pestellini & Aiello 1992; Zhu et al. 2014; Öberg et al. 2009b; Walsh et al. 2010, 2012; Bruderer 2013). The net surface area of dust grains within the rings is also much larger, which presumably fosters further volatile deposition and growth.

In this work, our goal is to understand the effect of a gap—ring substructure in the temperature and chemistry of a protoplanetary disk. We focus on the changes in the physical conditions inside the gap and the ring and how these changes lead to the given abundance and distribution of important chemical tracers.

This paper is organized as follows: Section 2 explains the setups of our thermochemical models, including the assumptions and testing goals. Section 3 shows the main results of the simulations, the chemical properties, and the synthetic ALMA images for a chosen set of molecular transitions. In Section 4, we discuss the possible implications of our results. Finally, we present a brief summary of this work in Section 5.

2. Modeling and Methodology

We study the chemistry and radiation fields in protoplanetary disks with a dust substructure, using the 2D thermochemical code rac2d (Du & Bergin 2014). The code calculates the dust thermal equilibrium with a Monte Carlo algorithm. After the thermal equilibrium is attained, the code iterates using chemical kinetics to reach a quasi-chemical equilibrium.

Our chemical network includes 484 species with 5830 chemical reactions. The gas reaction rates in the chemical network are mainly taken from the UMIST 2006 database (Woodall et al. 2007). Furthermore, the code includes reactions on the dust surface, which are taken from Hasegawa et al. (1992); the photodesorption of H₂O and OH by Lyα photons using yields from Öberg et al. (2009a); full Lyα radiation transfer and inclusion into photodissociation rates; and the adsorption/desorption of molecules on dust grains using the formalism as described in Du & Bergin (2014), which contains a thorough explanation of the code’s functioning.

The time evolution in rac2d is solved through logarithmic time steps in isolated cells. Our simulations do not take into account any turbulent mixing or radial motion in the gas or dust. During the chemical iterations, the code updates the heating/cooling sources in the gas, which allows us to find the gas temperature decoupled from the dust. The decoupling between gas and dust temperature becomes significant in the upper layers of the disk (Kamp & van Zadelhoff 2001; Jonkheid et al. 2004), where it is particularly important to make accurate predictions of the chemical rates and the molecular line emission in synthetic images.

Our goal is to analyze the effect of the gaps and rings on the chemical evolution of the disk. In order to do that, we include a static substructure in the density structure from the beginning of the simulations. Then, we observe how the substructure changes the final composition of the disk when compared with a disk model without them. The 2D nature of the code lets us analyze the vertical structure and the warm molecular layer as well.

Once we have run the simulations for 1 Myr, we compare our models, their thermal fields, and the distribution of molecules in the network, having a particular interest in the chemistry inside the disk substructure. Finally, we create synthetic ALMA images to predict how the local substructure within gas and dust alters the expected radial emission profiles.

2.1. Simulation Setup

Stellar irradiation is the main heating source of the disk, and along with the dust distribution, it sets the thermal profile of the disk. Likewise, UV and X-ray photons dominate the chemistry in the upper layers through molecular ionization and photodissociation.
Given that photodissociating photons play a considerable role in the disk chemistry, we use a large number of photon packages for the X-rays and the UV frequencies to minimize the photon noise in the Monte Carlo simulation. We run the simulations using $5 \times 10^5$ photon packages for the optical and longer wavelengths, but we include a refinement factor of $10^5$ for Ly$\alpha$ photons, $5 \times 10^5$ for UV photons, and $10^6$ for X-rays. By using the refinement factor, we increase the number of photon packages in the respective spectral window by the corresponding refinement value. Even using a refinement for the UV photons, the dust opacity does not let the UV photons reach the midplane. Nevertheless, the UV flux reaching the midplane and its associated photodissociation rate are negligible compared to the optical irradiation and the gas-phase chemistry, so it does not change our final results. Further, Agúndez et al. (2018) show that FUV photodissociation rates for T Tauri disks are negligible for $z/r < 0.3$ at 100 au.

In our basic or benchmark model, the surface density, $\Sigma_{\text{basic}}$, follows the self-similar solution from Lynden-Bell & Pringle (1974), i.e.,

$$\Sigma_{\text{basic}}(r) = \Sigma_0 \left( \frac{r}{r_0} \right)^{-\gamma} \exp\left[ -\left( \frac{r}{r_c} \right)^{2-\gamma} \right]$$

where $r_c$ is the radius of the exponential cutoff, $r_0$ is the characteristic radius for the disk, and $\Sigma_0$ is the surface density of the disk at $r = r_0$. In our basic model, the gas and dust components have the same profiles, where $\Sigma_0$ is the only changing value. For the disk with the dust substructure, we add the ring and the gap as modulations of the self-similar solution. Those modulations are further discussed in Section 2.1.1. We aim to include how the gas and the distinct dust populations alter the chemistry and physical conditions in the disk. So, we set different vertical distributions for them, but with the same functional form. Both gas and dust have vertical Gaussian distributions (Armitage 2010):

$$\rho(r, z) = \rho_0(r) \exp\left( -\frac{z^2}{2h^2} \right)$$

where $\rho_0 = \frac{\Sigma_{\text{basic}}(r)}{2\pi h}$ and $h$ is the scale height, which we vary for each population. Particularly for the gas, the aspect ratio is set to be $h/r = 0.08$ at $r = 100$ au. The scale height also has a radial dependence through a power law with a flaring index $\psi$:

$$h(r) = h_c \left( \frac{r}{r_c} \right)^\psi.$$  

The flaring index is a common value for the gas and dust populations. We set it with a value of $\psi = 1.22$.

Besides the gas, we include two main dust populations differentiated by the grain size they represent and an additional third component only within the inner 3.5 au. The two main populations are composed of a mixture of 80% silicates and 20% graphite. The optical opacities where taken from Draine & Lee (1984), while the X-rays opacities come from the prescription in Bethell & Bergin (2011). Both dust populations follow a grain size distribution with a standard power law, $n(a) \propto a^{-3.5}$, which is taken from Mathis et al. (1977). We also set a differentiated vertical distribution for different dust populations to consider the dust settling effect (Dullemond & Dominik 2004).

The first dust population is composed only of small grains ($0.005 \mu m < a_{\text{grain}} < 1 \mu m$). Although the small-grain population contains only 12.5% of the total dust mass, it has a considerable share of the total dust surface area in the disk, where most of the dust–gas reactions happen, and effectively governs the gas–dust interactions, except in the ring midplane. Given that the small grains are more coupled to the gas, we set an aspect ratio of $h/r = 0.08$ at $r = 100$ au for them.

The second dust population contains the large grains and the majority of the dust mass (87.5%). This population has a maximum grain size $a_{\text{max}} = 1$ mm and a minimum size $a_{\text{min}} = 0.005 \mu m$. The dust settling was implemented as follows: the large grains, which are more concentrated in the midplane, have an aspect ratio $h/r = 0.02$ at $r = 100$ au (Boehler et al. 2013). The settling becomes important for large grains because it changes the transparency to UV photons, producing a larger UV photon-dominated region. A UV photon-dominated region, along with the gap, could enhance the emission of small hydrocarbons (Bergin et al. 2016).

The third population has the same size distribution as the first one, but it is only composed of silicate grains in the inner 3.5 au. We are mostly focused on the gap at 100 au, but there is a transition in the dust composition inside and outside the water snow line, so we included the third population just for completeness.

The disk was modeled using a logarithmic grid in cylindrical coordinates $(r, z)$, with 300 cells in the radial direction between 0.1 and 300 au.

2.1.1. Disk Substructure

We include the gap—ring substructure by Gaussian modulations of the basic surface density profiles, locally increasing the amount of material. We use Gaussian profiles because, in contrast to step functions, they produce smooth transitions between the gaps/rings and the parametric surface density profiles of the disks. Despite that the sharpness of the feature will be dictated by the process forming it, the current spatial resolution precludes moving beyond a smooth Gaussian prescription.

1. Gap: We set the gap as a region where there is a local depletion of material for both dust populations and the gas. We characterize them by their location $r_{\text{gap}}$, the depth of the gap $\delta_{\text{gap}}$, and a width $w_{\text{gap}}$. In this case, we modulate the basic surface density using a Gaussian function:

$$\Sigma(r) = \Sigma_{\text{basic}}(1 - (1 - \delta_{\text{gap}}) \times \exp(- (r - r_{\text{gap}})^2 / 2w_{\text{gap}}^2)).$$

Thus, the location $r_{\text{gap}}$ sets the center of the material depletion, the depth $\delta_{\text{gap}}$ represents the ratio between the surface density in the center of the gap and the undepleted case, and the width $w_{\text{gap}}$ is the standard deviation of our Gaussian gap. It is noteworthy that instead of being absolute, the depth of the gap is relative to the surface density at that location in an undepleted case.

2. Ring: The ring is parameterized in a similar way to the gap, but the main difference is that it is an enhancement of material and it only applies to large grains (millimeter-sized grains). We only apply it to large grains because dust trapping is more efficient for larger sizes (Birnstiel et al. 2010; Pinilla et al. 2012; Weber et al. 2018).
Further, high dust density enhance dust growth, increasing the amount of large grains, while small grains are more coupled to the gas. By being more coupled to the gas, the small grains feel a stronger influence of the background gas pressure profile and thus do not form rings as readily as larger, less well-coupled grains do. Dullemond et al. (2018) showed that at current observational resolution dust rings can be modeled with Gaussian functions, so we use Gaussian modulation of the dust surface density to characterize the rings. Rings are characterized by their location $r_{\text{ring}}$, an amplitude $\delta_{\text{ring}}$, and a width $w_{\text{ring}}$. The final expression for the surface density including a ring is

$$\Sigma(r) = \Sigma_{\text{dust}}(1 + \delta_{\text{ring}} \exp(-(r - r_{\text{ring}})^2/2w_{\text{ring}}^2)).$$

A final summary of the parameters in our simulations can be found in Table 1. We based the main gap—ring substructure of our simulated disk on AS 209, which, besides having an axisymmetric dust emission with a large gap, has been previously modeled with a giant planet carving the gap (Salyk et al. 2013; Banzatti et al. 2017; Avenhaus et al. 2018; Fedele et al. 2018). However, even though the actual parameters of the substructure will depend on the conditions of each particular disk and the planet creating the substructure, its functional form is rather generic (Dong & Fung 2017; Zhang et al. 2018). Despite that we based our model on AS 209, instead of making a source-specific model, we explore the effect of the substructure on the thermochemical structure of the disk. Small grains and gas have a less depleted substructure than large grains as they couple to the gas. Large grains are not dynamically coupled to the gas, so they get trapped in the pressure maxima at the gap’s edge. The aim is to find the physical conditions produced by such substructure on the disk and the chemical networks that it could trigger. Thus, we use different depletion factors for small and large grains. We used a depletion for large grains similar to the one used by Facchini et al. (2017), while our gas and small-grain depletion is similar to the value used by Favre et al. (2019) (see Table 1).

We illustrate how the substructures change the surface density profile in Figure 2. We also show the vertical density distribution for the gas and the two main dust populations in Figure 3. The figure shows the dust settling in large grains and how the gap—ring substructure differs from the basic model. The gap lies at 100 au, and the ring is placed at 120 au.

### 2.1.2. Initial Chemical Abundances

The initial abundances set the stage for the overall chemical evolution and are given in Table 2. The elemental abundance for C, H, O, and N is within the range of the reported abundances in the literature for the interstellar medium (ISM; Nieva & Przybilla 2012). At the beginning of our simulations we set CO as the main carbon carrier. The disk shields itself to UV photons with enough energy to photodissociate CO, which implies that at the beginning of the disk the carbon available will react with the oxygen to create CO (Langer 1976). We chose to put the CO in the gas phase because the binding energy of CO is low enough for several desorption mechanisms to be effective in keeping the bulk of CO in the gas phase (Bergin et al. 1995).

Given that we set the oxygen to be more abundant than carbon in our simulations ($C/O \sim 0.4$), the remaining oxygen will react to create water. Even though it is pressure dependent, the sublimation temperature of water is above 100 K (Bergin & Cleeves 2018), which is usually located within the inner few au for the midplane (Lecar et al. 2006). Hence, we choose to input the water as ice; otherwise, it would immediately sublime beyond or above the snow line.

Nitrogen is initially presented in its atomic gas form. The initial form of nitrogen is actually uncertain, but Schwarz & Bergin (2014) show that nitrogen being initially present in its atomic form is the best match for the current ammonia-to-water ratio in comets.

Heavy elements are important for the ion balance given that they exchange charge with other molecules and have longer recombination timescales, so they stay charged longer. Early work suggested that these species are depleted in the dense ISM, and we adopt that conclusion as well (Graedel et al. 1982).

### Table 1

| Parameter | Value |
|-----------|-------|
| Disk mass | $70 M_{\text{Jup}}$ |
| Dust mass | $0.8 M_{\text{Jup}}$ |
| Stellar radius | $2.4 R_{\odot}$ |
| Stellar mass | $0.9 M_{\odot}$ |
| Stellar temperature | 4250 K |
| UV luminosity | $2.91 \times 10^{32}$ erg s$^{-1}$ |
| X-Ray luminosity | $3.69 \times 10^{30}$ erg s$^{-1}$ |
| $T_{\text{X-Rays}}$ | $10^7$ K |
| Ionization rate | $1.36 \times 10^{-17}$ s$^{-1}$ |
| $\tau_{\text{disk}}$ | 1 Myr |
| $\gamma$ | 1 |
| $\psi$ | 1.22 |
| $r_c$ | 100 au |
| $r_{\text{gap}}$ | 100 au |
| $\delta_{\text{gap,large dust}}$ | 0.0025 |
| $\delta_{\text{gap, gas}}$ | 0.085 |
| $w_{\text{gap}}$ | 16 au |
| $\delta_{\text{ring}}$ | 120 au |
| $\delta_{\text{ring}}$ | 26 |
| $w_{\text{ring}}$ | 4.11 au |

### Figure 2

Surface density of a modeled disk including the dust substructures. The gap is modeled as a depletion of material in gas and dust, while the ring is an enhancement or dust trap only in the dust large grains. It is noteworthy that the gap has different depletions for small and large grains, as larger grains would be less coupled to the gas. The gap and the ring were modeled using Gaussian modulations of the undepleted surface density $\Sigma(r)$, shown with dashed lines.

The initial form of nitrogen is actually uncertain, but Schwarz & Bergin (2014) show that nitrogen being initially present in its atomic form is the best match for the current ammonia-to-water ratio in comets.
2.2. Image Creation

We create synthetic images assuming a distance of 125 pc and a face-on orientation \((i = 0^\circ)\). The face-on orientation removes systematic degeneration in the ray-tracing and allows us to trace better the emission layer of a given line. We produced spectral cubes containing dust continuum and molecular line emission. We convolved the spectral cubes with circular Gaussian beams. We focused on emission falling within Band 6 of ALMA \((211 - 275 \text{ GHz})\), observed with an angular resolution of \(0''.1\) (12.5 au at a distance of 125 pc). We generated cubes with a spectral resolution of 0.01 km s\(^{-1}\), which are then convolved to a 0.1 km s\(^{-1}\) spectral resolution. By using that initial spectral resolution, we avoid artificial error produced in the image from the ray-tracing that samples specific frequencies rather than a frequency bin. We only report the moment 0 maps corresponding to the integrated intensity.

Finally, we subtract the dust continuum emission by interpolating a linear function using the values at the two extremes of the spectral cube.

3. Results

In our analysis, we compare the difference between the outputs of the fiducial model without any substructure and the model that includes the presence of the gap and the ring. We contrast the physical and chemical structures derived for both models.

3.1. Physical Conditions

3.1.1. Radiation Fields

We show the changes in the radiation fields due to the dust substructure in Figure 4. Dust depletion inside the gap decreases the optical depth to high-energy photons. UV radiation thus penetrates deeper and closer to the midplane in the gap, and to a less extent X-rays. In contrast, high-energy photons cannot penetrate inside the ring owing to the high concentration of dust. We zoom in inside the dust substructure and compare the ratio of the UV fluxes in our two models in Figure 5. The figure shows that the UV flux is mostly enhanced in the back of the gap, probably due to back-scattering. It is worth mentioning that the UV flux at deep layers is much lower than on the surface. Thus, even if the UV flux near the midplane is increased by a factor of a million, it does not imply that the UV is actually higher than in the surface. It only states that the UV photons penetrate deeper when a gap has been carved.
The change in X-ray flux is less strong than in the UV. Even though the X-ray flux increases in the gap and in the layer immediately above it, the X-ray ionization rate is low enough that it will not be the main driver of the chemistry in those deep layers (depending on presence/absence of cosmic rays). The shielding effect of the ring in the X-rays is also present, as the midplane effectively has zero X-ray flux and ionization. This is because the higher dust density increases the availability of readily absorbing Fe, Mg, Si, and O atoms. This absorption is more closely concentrated toward the midplane than for UV owing to the extra penetration power of X-ray radiation. Kim & Turner (2020) show that the X-ray flux increases inside gaps. Our results have a less prominent X-ray flux increase, mainly because their models have a harder X-ray spectrum with X-ray photons at a higher frequency.

This has the effect of increasing the ionization level, because the efficiency of the scattering of X-rays by dust grains is proportional to the energy of the X-ray photons (Bethell & Bergin 2011) and there is greater penetration power (Igea & Glassgold 1999). A harder X-ray spectrum will result in a more significant level of back-scattering from the outer wall of the gap, increasing the X-ray flux within the gap.

3.1.2. Thermal Structure

The thermal structures of the gas and the dust have significant changes in the gap and ring. Teague et al. (2017), van der Marel et al. (2018), and Facchini et al. (2018) have looked at the thermal fields inside the dust substructure, although they obtain different results; such differences will be discussed further in Section 4.3. In our models, there is a noticeable cooling effect at the ring location, where the gas and dust temperatures decrease by more than 5 K. That slight change becomes significant when compared with the expected temperature from the basic model, which is slightly below 20 K. On the other hand, the dust temperature is slightly increased in the gap. In Figure 6, we take the difference between our two models to isolate the change induced within the gap/ring. Here we observe a dust temperature increase of almost 5 K within the gap and a decrease of 10 K in the ring. The effect is caused by the change in the overall opacity to the stellar irradiation and high-energy photons. Inside the gap, the optical and UV photons will reach deeper and closer to the midplane, having a net heating outcome. The opposite effect is observed in the ring, where dust grains shield themselves and the gas to the general radiation, particularly in the midplane, meaning that the optical depth is increased, so optical and UV photons are not able to reach inside the ring.

In the upper layers of the atmosphere, we also observe a slight increase in temperature. We associate it with the fact that photons in the upper atmosphere are able to reach farther distances in the disk, due to the depletion of material in the gap,
which reduces the line-of-sight optical depth, measured from the star.

The disk is optically thin to UV and optical radiation in its higher layers. However, the significant changes to the optical depth occur deeper in the disk, closer to the midplane as is observed in Figure 7. The figure shows vertical thermal cuts in the disk for both the gap and the ring and how they diverge at lower heights. The thermal influence of the gap–ring substructure in the dust is produced closer to the midplane ($z/r < 0.1$), where the dust mass is concentrated, rather than the dust-depleted disk surface. In terms of the net temperature variation, the thermal change in the ring is more significant than the increase of temperature in the gap.

3.2. Chemistry in Gaps and Rings

3.2.1. Radial Abundance Structure

We show the different profiles comparing the impact of dust substructure in Figure 8. Each abundance was obtained by dividing the column density of a given species by the total number of gas particles at a given radius, i.e.,

$$X_i(r) = \frac{\int X_i(r, z)n(r, z)dz}{\int n(r, z)dz},$$

with $X_i(r, z)$ the abundance of a given species at a given $r$ and $z$, and $n(r, z)$ the gas number density field.

If we focus only in CO, we observe that the CO ice sublimates in the gap, but there is also chemical reprocessing, such that the carbon in the gas phase within CO is transferred into CO$_2$ ice on the grains. Thus, the C atoms that would be frozen on the grains are now divided between volatiles species (CO) and the grains (CO$_2$), even for a gap located at 100 au. Inside the gap, the volatile CO increases its abundance by more than one order of magnitude, fully compensating for gas depletion inside the gap in this case. However, there is an interplay between the depth of the gap and its physical conditions. This leads the CO abundance increase to be concentrated near the midplane and not distributed vertically within the gap, as seen in Figure 9. In this particular model the gap is located beyond the CO sublimation front, so CO will be predominantly found in the warm molecular layer of the gap that is above the vertical CO snow line (Aikawa et al. 2002). CO sublimation in the gap occurs close to the midplane driven by thermal and photodesorption, making the CO more concentrated below the vertical CO snow line of the undepleted case, as is shown in Figure 9.

The CO in the ring does not show strong trends, although the carbon gets transferred to different carriers. The frozen CO does not show strong changes; however, hydrogen cyanide (HCN), a nitrogen compound, becomes a main carbon carrier. The main carbon carriers and the related chemistry are presented in Section 3.2.3. The middle panel of Figure 8 illustrates how the dust substructure shifts the carbon carriers in the dust grains. The main carbon carrier in the midplane at 100 au shifts from CO to CO$_2$, where the CO in the grains gets oxidized to create CO$_2$, to the detriment of the CO abundance. Nevertheless, in the very center of the gap, where the temperature is the highest and the optical depth the lowest, gas-phase CO still remains the dominant carbon carrier. The increased rate of photodissociation, higher temperature, and lower density counteract the formation of CO$_2$.

The last panel in Figure 8 shows photochemical tracers in the disk, C$_2$H and HCO$^+$. C$_2$H is an important tracer of the UV-driven chemistry and also of the $\tau_{UV} = 1$ layer (Henning et al. 2010). C$_2$H also responds to the CO distribution, such that it is abundant right above the CO self-shielding layer. We would expect that since the penetration of UV photons is deeper in the gap, the abundance of C$_2$H, a photochemical tracer, might be enhanced. Figure 8 shows a peak in the C$_2$H and HCO$^+$

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**Figure 6.** Thermal structure of dust and gas including the gap and the ring in the disk profile. Top: dust and gas temperature in the disk from left to right. It is observed that the ring is noticeably colder, while the gas is particularly hotter in the gap. Bottom: difference in temperature between the disk model with the dust substructure and the same disk model but without the substructure. It shows that the gap in both cases could be hotter, up to more than 5 K, while the ring is much colder, by almost 10 K.
molecules like CO. In temperature in the gap is smaller, it could be enough to thermally desorb
the center of the gap. Bottom: vertical cut at 120 au in the center of the ring. They
comparing it with a model without them. Top: vertical cut at 100 au in the
abundances inside the gap. The increase in C2H abundance
could lead to the formation of HCO$^+$.

Figure 7. Vertical cut of the thermal field in the middle of the gap and the ring
comparing it with a model without them. Top: vertical cut at 100 au in the
center of the gap. Bottom: vertical cut at 120 au in the center of the ring. They
both show that the change in temperature happens within one scale height ($r_c/r < 0.08$), where the ring gets colder by more than 5 K. Even if the increment in temperature in the gap is smaller, it could be enough to thermally desorb molecules like CO.

abundances inside the gap. The increase in C$_2$H abundance
associated with the gap is compensated by the depleted gas
surface density. Such interplay between abundance and surface
density causes C$_2$H to have a broad flat distribution—notably
not a decline in emission given the drop in the overall surface
density. The predicted vertically averaged abundances in this
model are quite low, and below what is inferred from observations of \( \sim 10^{-7} \) (Bergin et al. 2016; Bergner et al. 2019). The UV field inside the gap is favorable for the production of C$_2$H. However, in order to increase the C$_2$H abundance, a C/O ratio higher than unity is needed; otherwise, CO will be carrying most of the carbon content in the substructure (Bergin et al. 2016; Kama et al. 2016; Miotello et al. 2019). Therefore, a carbon source inside the gap is necessary to locally increase the C/O ratio, which in turn will enhance the C$_2$H abundance. Some possible carbon sources in the substructure will be further discussed in Sections 4.1.2 and 4.4.

In addition to C$_2$H, we show HCO$^+$, which forms via X-ray ionization on disk surfaces (Semenov et al. 2004; Clevees et al. 2015). Regarding a photochemical tracer more sensitive to X-rays, HCO$^+$ abundance also increases in the center of the gap. The HCO$^+$ increase is due to the CO sublimation right in the center of the gap, which is one of the main species that could lead to the formation of HCO$^+$ through the reaction of H$_2$ and CO. In the colder outer regions, even though X-rays and cosmic rays have a higher mean free path, HCO$^+$ is less abundant because it recombines, transferring the carbon to other molecules such as CO, CO$_2$, or H$_2$CO.

In general, we find that the ring at 120 au is not favorable for the production of photochemical tracers. The dust enhancement within the ring shields the midplane from high-energy radiation and ionization. However, the ionization rate in the midplane is already low in the undepleted case; the addition of a substructure produces an even lower abundance of photochemical tracers. Therefore, the ring does not have an observable effect in the disk photochemistry. However, the ring is colder and, depending on the location with respect to the star, may provide an enhanced site for molecular freeze-out (e.g., Krijt et al. 2016), which leads to localized ice enhancements.

3.2.2. Vertical Shift of the Warm Molecular Layer

We observe that with the inclusion of a gap in the gas and dust the disk becomes “chemically thinner.” It is chemically thinner in the sense that the warm molecular layer has a vertical shift to a lower layer closer to the midplane, as can be observed in Figure 10. The warm molecular layer (Aikawa et al. 2002) is the visible gas-phase chemistry layer in the disk where CO sublimes at \( T_{\text{dust}} > 20 \) K (Bergin & Cleeves 2018) and the UV optical depth exceeds unity, i.e., molecular photodissociation becomes less important. This layer generally resides in the disk surface layers as seen in our fiducial model (Figures 9 and 10). In the case of a disk with a gap, this layer shifts deeper in the disk closer to the midplane as shown in Figure 10. This suggests that there is a chemically active layer closer to the expected location of protoplanets driving the gap formation. Under strong levels of vertical mixing, the shift could be significant enough to ease the transport of volatiles between the warm molecular layer and the protoplanet at the disk midplane.

At the location of the ring, given that the disk is colder, most of the molecules are already frozen. Therefore, there is no apparent shift of the warm molecular layer. However, if the ring were located closer to the star, it is possible that this conclusion could change. The role of the ring for terrestrial seeds would be the opposite to the giant planet that carved the gap. The warm molecular layer could potentially be pushed to higher altitudes. The colder temperatures in the ring would then enhance the freeze-out of certain species in a location that is potentially the next site of planetesimal formation.

3.2.3. Carbon Carriers

We show the main carbon carriers (species carrying the highest number of carbon atoms) at each location in Figure 11. The primary change is the enhanced presence of CO closer to the midplane within the gap (i.e., the shift of the warm molecular layer). This also produces a localized change in the C$+$/C/CO transition zone.

Regarding the solid ices within the disk, an important phenomenon is the photodissociation and photodesorption of water molecules through the UV field induced by cosmic rays, which takes place in the midplane. The photodissociation of water inside the gap generates an OH radical that reacts with CO on the grains forming CO$_2$ ices. Therefore, CO$_2$ becomes the main carbon carrier at those layers. However, this outcome is dependent on the local C/O ratio and water being dissociated to oxygenate the medium. The enhancement of CO$_2$ is seen in Figures 8 and 9.

Inside the ring, instead of H$_2$CO being the main carbon carrier at that region, as seen in the baseline model, we see a
Figure 8. Abundance radial profiles for different species of interest in a disk with the gap and the ring (left) and the benchmark without them (right). Top: CO radial profile showing its sublimation into the gas phase inside the gap. CO abundance increases by an order of magnitude at the inner edge of the gap because of CO thermal desorption. Middle: carbon carriers in dust grains in the ring and the gap. The shifting between CO and CO$_2$ in the grains caused by the water dissociation and the subsequent reaction between CO and the OH radical is noteworthy. Bottom: photochemical tracers that show the change in opacity to high-energy photons in the gap and in the ring.

Figure 9. Comparison of the abundances of certain species of interest for a disk with the gap—ring substructure and the benchmark. Left: 2D abundances in the disk model including the dust substructure. Right: 2D abundances in the disk without dust substructure. The zoom-in shows the gap location. The zoom-in illustrates the CO sublimation in the gap, in particular at the inner edge of the gap. It also shows the production of frozen CO$_2$ in the grains right above the midplane for the model with the dust substructure. Water is being desorbed and photodissociated, which liberates an OH radical that will oxygenate the chemistry. Overall, the gap and the ring have the power to increase or decrease the abundance or molecules of interest in orders of magnitude, which should be taken into account for the observation of line emission.
A significant amount of C and N within HCN. To make HCN the main carbon/nitrogen carrier, the chemical path taken is through the reaction between frozen nitrogen and CH. The nitrogen comes from a gas-phase reaction of the ammonia cation, NH\(^+\), with molecular hydrogen that freezes out, while the CH is produced by photodissociation of small organics. In other words, the low temperature in the ring, along with cosmic rays, allows the sublimation of nitrogen and the photodissociation of small organic molecules, producing HCN on the surface of the dust grains.

### 3.3. Observational Predictions

The sublimation of CO in the midplane inside the gap will change the emission of CO and its isotopologues. If the gap is not deep enough, CO emission changes from an optically thin regime in an undepleted disk to an optically thick regime in the disk with the gap, an effect that has been reported by van der Marel et al. (2019) and Facchini et al. (2018). However, whether or not the CO emission is increased locally is dependent on the excitation conditions in the gap, specifically the local density and temperature.

We create synthetic images for the CO and its \(^{13}\)CO and C\(^{18}\)O isotopologues in the \(J = 2\rightarrow 1\) transitions at 0.
°1 resolution, observable in Band 6 of ALMA (211–275 GHz). We show the integrated intensity images and their respective CO column density and emission radial profiles in Figure 12. Our predictions show that for a gap with the chosen depth, the emission at the location of the dust substructure is lower, but the overall emission does not correlate with the depth of the gap or the CO column density. The gas depletion is 92% of the undepleted value, i.e., \(0.08 \cdot \Sigma_{\text{basic}}(r)\), but even if the CO emission does decrease significantly, it is less than a factor of 2. In this regard, there are two effects that are relevant toward the emission, as the higher temperature tends to increase emission in specific rotational states, while the gas density decrease in the gap would lower emission. In order to disentangle the effects of gas density and temperature on CO emission, the thermal structure of the disk is needed. This effect has been previously discussed by Facchini et al. (2018) in a gap in the inner disk at \(\sim 20\) au. In our model, for optically thin lines, the depth of the gap in emission is less than that within the H\(_2\) gas itself. CO sublimation inside the gap counters gas depletion, which is particularly relevant beyond the CO snow line.
Among the different CO isotopologues, the less abundant isotopologues are better tracers of the gap chemistry. Given that they have relatively lower optical depth, they trace deeper layers closer to where the CO desorption front is located in the gap. However, the gas temperature in the midplane of the gap, even if elevated, remains colder than in the upper layers.

Figure 12. Synthetic images for CO $J = 2–1$ transition with $0''/1$ resolution. We show the radial profile of the integrated intensity in blue and the radial profile of column density for the respective CO isotopologue in purple. Top: $^{12}$CO. Middle: $^{13}$CO. Bottom: C$^{18}$O. The radial profiles show a dip in the gap for $^{12}$CO, the optically thick tracer. On the contrary, the emission peaks for the optically thin ones, and then it decreases in the ring. In particular for CO in the gap, it will be concentrated in the midplane, which is colder than the upper layers, so its emission will be lower for $^{12}$CO, which is optically thick, but it will be higher for $^{13}$CO and C$^{18}$O due to the fact that they are in the optically thick regime. However, because the increase in CO abundance is coming from deeper and colder layers of the disk, the increase in CO emission is small. The different consequences of the substructures in the line emission of CO show a degeneracy between the column density (disk mass+abundance) and the depth of the substructure.
surrounding the gap. To distinguish these differences requires high resolution and sensitive observations.

### 3.3.1. Effect of Disk Masses

In order to test the possible effect of disk mass on the overall chemical distributions, we explore a simulation that increases the gas and dust mass by a factor of 10. In this model we keep the same relative gap depth and ring enrichment. Even though the actual material depletion is different in absolute terms, the gaps carved by planets are dependent on the host disk properties and will scale with the surface density profiles (Duffell & MacFadyen 2013; Fung et al. 2014; Duffell 2015).

The comparison that is seen in Figure 13 shows that for a very massive disk the $^{12}$CO emission, while showing slightly different structure, has only a small change compared to the order-of-magnitude increase in the CO content. The radial profiles of $^{12}$CO emission show that the dip in the gap is shallower for the massive case. We associate the change in the trend with the fact that $^{12}$CO remains optically thick in the massive disk, while in the hotter, less massive disk, the $^{12}$CO becomes optically thinner inside the gap, tracing deeper and colder layers. A similar behavior can be extrapolated to the other CO isotopologues, where the emission becomes comparable inside the gap. Therefore, the actual dip in the CO emission is related to the gas surface density and the traced layer, where an excitation temperature effect can be observed as well.

### 3.3.2. Effect of Different Cosmic-ray Ionization Rates

Cosmic rays are one of the main heating sources in the midplane, particularly at large radii. We explore the effect that cosmic rays have in our models. Since cosmic rays can reach deeper layers in the disk, they cause the dissociation and desorption of several species, and they also ionize the medium, enriching the reactions of photochemical tracers such as HCO$^+$ and H$_2$CO. We can see in Figure 14 that when cosmic rays are removed, there is less CO desorption; however, it is still present, in particular at the deepest point of the gap. Even if CO and H$_2$O are desorbed, they do not photodissociate in the midplane. On top of that, we expect that the presence of cosmic rays will enhance the production of methanol (CH$_3$OH), becoming one of the main carbon carriers as the bulk chemistry evolves from small organics toward more complex molecules.

### 4. Discussion

In general, our results suggest that the gap carved by the planet has a different thermal structure than in the undepleted case, with a different radiation field as well. Given that the $\tau_{UV} = 1$ layer is pushed closer to the midplane (see Figure 1), if the planet gets massive enough, UV photons could even reach the midplane. We therefore expect more chemical interaction between the planet and the warm molecular layer, along with a higher ionization fraction around the planet. Such interaction would be enhanced with more massive planets.

It is still a matter of discussion whether planets are the ones carving the gaps and creating the rings, or planets are being formed on those regions. However, the link between dust substructures and the changes in the physical and chemical structure of the disk they incite is a vital relationship to understand.

#### 4.1. Physical Structure

The actual effect of the dust substructure will be dependent on the dynamical structure and properties of the host disk and on the substructure itself. Nevertheless, our model is a reasonable starting point and allows us to qualitatively understand the general impact of a dust substructure on a protoplanetary disk.
4.1. Location and Depth of Dust Substructure

In our models we have explored the chemistry inside a gap—ring substructure at one location beyond the CO snow line in a young disk. If the gaps/rings are situated closer to the star, more volatiles would be present, enhancing photoprocessing in the gap, while within the ring, denser conditions would enhance any freeze-out. If the substructure were farther out in the disk, the ring would induce a less noticeable effect, but the gap could increase the sublimation of molecules through photodesorption.

We predict that the depth or strength of the substructure is also important for the warm molecular layer shifting deeper into the disk. A deeper or more dust-depleted gap would increase the transparency of the gap to UV photons, placing the gap in the disk. A deeper or more dust-depleted gap would also be important for the warm molecular layer shifting deeper into the disk. A central question for later exploration will be whether the gap is inside or outside the snow line, the location of key volatile ices in the midplane, such as CO, CH₄, and CO₂.

4.1.2. Meridional Flows and Mixing

Several 3D hydrodynamical simulations show the presence of vertical flows inside the gaps carved by massive planets (Morbidelli et al. 2014; Fung & Chiang 2016; Szulágyi et al. 2016). These vertical flows, labeled meridional flows, move gas and small dust from the surface of the disk toward the midplane inside the gap and upward inside the disk beyond gap edges. Meridional flows have been observationally confirmed by Teague et al. (2019) and may therefore change the chemical composition of the gap as seen in our simulations. The observational effects of such flows on the chemical properties of the gap are uncertain. However, Szulágyi et al. (2016) show that planets accrete through inflows with significant vertical components. A strong vertical component in the accretion inflow implies that the planet’s composition could be enriched with the chemically active layer above and below it, an effect that has also been explored by Cridland et al. (2020). A thorough description of meridional and radial flows in planet-forming regions is beyond the scope of this paper. However, we run 3D simulations with the hydrodynamical code PLUTO (Mignone et al. 2007) to test and to obtain order-of-magnitude values for the mass flows in the substructure (see Appendix).

Based on our simulations, we expect radial mass flows in the midplane going away from the planet to be of the order of 10−100 M⊙/Myr−1. Therefore, there is some mixing between the gaseous CO in the warm molecular layer and the midplane in the gap via vertical flow, and from the midplane to the gap’s edges via the radial component of the motion. Thus, both dissociated photoproducts of gas and ice, along with shielded molecules and ice-coated grains, will flow toward the midplane.

Further, the gaseous species that settle into the midplane but not onto the planet would be pushed toward the gap’s edges (see Kley 1999 for the velocity flow field inside the gap). The species drifting to the inner edge either will follow the gas flow, returning to the midplane chemical equilibrium, or will get trapped in an inner dust-rich ring. In the outer edge the volatiles may be photodissociated by the UV back-scattering as they flow toward the outer pressure maxima, where the ring is present. Figure 15 shows how the surface area increases by two orders of magnitude between the gap and the ring. Throughout much of the disk, the surface area of solids is dominated by more numerous small grains; however, in the ring the probable dust growth, dust settling, and therefore pileup of large grains may lead the millimeter-sized particles to have a bigger share of the dust grain surface area, nₚσ. Thus, the ring, which is also locally colder, presents a freeze-out trap for this flow, and all volatiles in the gas will likely be deposited on grain surfaces. This will produce local enrichments of volatiles into ices depending on the overall temperature of the ring. However, whether this is a dominant effect is still unknown. Among the species enriching the dust grains, we expect gaseous CO or C atoms to be present, which increases the C/O ratio within solids in the ring. This effect is important, as the dust-rich rings represent likely sites for subsequent rounds of planetesimal formation and icy/rocky planet growth.

4.2. Observational Footprints of the Dust Substructure Properties?

Gas line emission is a central method to probe the physical properties within gaps and rings. Due to their abundance and subsequent emission brightness, CO isotopologues are main molecular tracers used to measure disk gas column density and temperature structure. However, chemical effects in planet-forming regions, i.e., inside dust substructures, change the relative abundance of CO to H₂, which leads to inaccurate measurements of the gas surface density. For example, ¹²CO emission is optically thick in general disk gas and is therefore a preferred temperature tracer (Beckwith & Sargent 1993; Schwarz & Bergin 2014; Weaver et al. 2018). In our simulations, the emission of ¹²CO coming from the gap is decreased by less than a factor of two (see Figure 12), but the actual gas surface density is decreased by an order of magnitude. Thus, the emission of ¹²CO keeps being optically thick, and it is not a reliable tracer of the H₂ column density.
This effect has been explored in more detail by van der Marel et al. (2019). They show that the actual trend in the CO emission and its isotopologues has a strong dependence on the depth of the gap.

Despite that $^{12}$CO by itself does not trace all the physical conditions in the disk, by using different CO isotopologues and other chemical tracers, we can discern the degeneracy between the chemistry and the physical conditions in the disk. Because CO isotopologues trace different layers within the disk, observing them gives us a first approach to the disk vertical structure. However, such an approach is not enough given that they do not give the full chemical picture of the disk. The abundance of different molecular tracers is susceptible to local radiation fields and the relative abundances between volatile elements, such as C$_2$H and HCO$^+$. To summarize, more than one molecular line is necessary to have a full thermochemical description around the planet-forming regions in a protoplanetary disk.

4.3. Comparison with Previous Models Present in the Literature

There are previous works in the literature simulating the effect of dust substructures on the chemistry of protoplanetary disks and the respective line emission predictions. For instance, Facchini et al. (2018) agree with some of our results in terms of the radiation field increasing inside the gap. In their simulations, they locate a planet carving a gap at 20 au, including the 1D dust evolution code from Birnstiel et al. (2010), which sets the dust size distribution and surface density in the substructure. They find that the $T_{\text{gas}}/T_{\text{dust}}$ ratio decreases in the gap, particularly in the midplane. Their result differs from ours, because their modeled dust-to-gas ratio inside the gap is lower. With such high dust depletions, the gas and the dust are not thermally coupled, leading to an increase in the dust temperature, while the gas is colder. Also, in our model we fixed the vertical structure to account for dust settling. Compared to Facchini et al. (2018), the dust-to-gas ratio in our models will be higher in the gap, and particularly in the midplane, leading to the differences in our thermal structure.

Van der Marel et al. (2018) study the CO emission for gaps created by snow lines or carved by planets. They illustrate the effect that different gap depths would have on the emission profiles of CO isotopologues. In terms of the physical properties, their models have assumed dust and gas depletions that encompass our baseline model. In their modeling, the dust and gas temperatures are still coupled in the denser layers of the disk, and they predict a higher UV flux in the gap as well, although they do not have a ring in the models. They show that the CO emission inside the gap could increase or decrease depending on the depth of the substructure. Both van der Marel et al. (2018) and our model predict CO sublimation in gaps beyond the CO snow line. In order to probe the actual depth of the gap in the gas surface density, one must move toward a larger variety of molecular species to characterize such substructures. Thus, more information about the thermochemical and dynamical structure of the disk is needed.

A previous model by Favre et al. (2019) focused on the same source has similar effects to the ones reported by us. A CO abundance enhancement inside the gaps is also observed, at least for the two most abundant CO isotopologues. Our simulations do not include isotope-selective photodissociation, which explains why their C$^{18}$O abundance decreases inside the gap. Their CO abundance agrees with our findings. Even considering the gas depletion inside the gap, the CO column density drop is not as significant as the gas surface density with a higher CO abundance.

4.4. Limitations of Our Simulations

Our thermochemical runs assume several simplifying assumptions. We only consider a static structure. Thus, any dynamical evolution of the disk has not been taken into account. The main carriers of molecules through the disk will be micron-sized dust grains and millimeter-sized pebbles. As pebbles drift, they would carry frozen molecules across the snow lines, changing the local composition and enriching the chemistry, mostly in the inner 10 au of a protoplanetary disk (Booth & Ilee 2019), or even further for hotter disks.

The static structure of our model does not include the drift of small grains onto the gap and the subsequent carbon grain destruction. The carbon grain destruction could be relevant if we consider the drifting of grains from the outer disk that could enrich the gaseous carbon chemistry inside the gap. Wei et al. (2019) show that carbon grain destruction would replenish the gas chemistry with carbon, while the oxygen gets frozen out. However, they explore the region inside the inner 10 au. Nevertheless, carbon grain destruction can increase the C/O ratio, generating a more carbon-driven chemistry, which may change the main carbon carriers inside the substructure and the CO abundance as well.

We only located the gap in one location, so its effect on the chemistry is dependent on the species present there. Further, the gap location with respect to the snow-line location of key volatiles (e.g., CO or H$_2$O) should have significant differences, as the physical local conditions and chemical species present differ between snow lines. Such differences have not been explored in detail and would give us insights about the chemical differences between planets formed at different locations.

5. Summary

In this study we modeled the chemical evolution in a protoplanetary disk by adding a gap and a ring as dust substructure in the density profile of the disk. We found different effects on the disk physical and chemical conditions:

1. Where the disk is depleted in gas and dust, i.e., inside the gaps, it becomes more transparent to radiation, therefore heating up that region. At the same time, high-energy photons (UV and X-rays) penetrate deeper in the disk, so the photochemistry is enhanced at the gap. One key effect is back-scattering off the outer edge of the gap.
2. In the rings or dust-rich regions, the disk is shielded to radiation and high-energy photons and becomes relatively colder. The rings present a freeze-out trap for the molecules that would otherwise be in the gas phase, i.e., rings have the potential to lock up some volatile species on the grains.
3. Since the disk inside the gaps is more transparent, the UV photons and the cosmic rays will push the molecular layer closer to the midplane. Inside the gap, CO sublimation in the midplane from residual small grains that drift inside the gap increases the amount of gaseous CO in the locations of planet formation. Cosmic rays, if present, enhance the production of CO$_2$ on the grains, rather than
locking up the carbon atoms in other molecules. Molecular tracers of X-rays and UV radiation, such as HCO\(^+\) and C\(_2\)H, will also be produced, particularly in the middle of the gap, although we predict that it will depend on the gap’s relative depth and the X-ray flux in the disk.

4. The dust grain surface area in the rings is larger by almost two orders of magnitude. Therefore, the gas-grain chemistry will be more important considering the freeze-out of gaseous molecules due to the lower temperature in the ring.

5. The observational effect of the gap will be degenerated with its depth. Even if the local abundance of gaseous species is increased, their column density will be dependent on the local gas surface density. On top of that, most of the gas species are desorbed closer to the midplane. Given that the temperature in the midplane is usually lower than the one on the surface, the actual line emission may be lower, which could lead to a misinterpretation of gas depletion inside the gap.

6. The meridional flows in the disk are fast enough to carry the sublimated species in the gap toward its inner and outer edges. The meridional flow on top of radial flows in the midplane chemically enriches the dust grains and pebbles located at the edges of the gap. Such pebbles and dust grains are considered seeds for rocky cores that may end up forming a planet.

7. Although our simulation put the substructure in only one location, we expect its influence on the chemistry and the physical conditions to be significant. Nevertheless, its effect may vary depending on where it is located.

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Software: Astropy (Astropy Collaboration et al. 2013, 2018), rac2d (Du & Bergin 2014).

Appendix A
Hydrodynamical Tests

In order to get approximated mass flow values in the dust substructure, we run hydrodynamical simulations with PLUTO (Mignone et al. 2007). We consider a 0.09 Jupiter mass planet at 100 au and an \(\alpha\)-viscosity, \(\alpha = 10^{-5}\), following a similar setup to that used by Zhang et al. (2018) to fit the dust continuum emission of AS 209, although with a higher viscosity. The simulation runs for 1000 orbits, equivalent to 1 Myr with a planet at 100 au. After the 1000 orbits, the mass flows were calculated. As result of the vertical shear of the disk setup, the isothermal equation of state, and the low \(\alpha\)-viscosity set in our simulations, there is a significant influence from the vertical shear instability (Nelson et al. 2013) in the mass circulation of the disk.

In Figure 16 we show the azimuthally integrated radial and meridional flows, \(\int\rho v_r r^2 \, d\phi \, d\theta\) and \(\int\rho v_r r^2 \, d\phi \, dr\), respectively. We observe that the radial flow of mass in the midplane at 100 au is \(~\sim 50 M_\oplus\) Myr\(^{-1}\). With such a mass flow rate, in 1000 yr, the CO photodissociation timescale in the gap, a mass of 0.05 \(M_\oplus\) would move out of the gap. Therefore, the radial circulation in and out of the gap allows the chemical enrichment of the dust grains and dust grains located at its edges. The chemical species with large timescales \((\tau > 10^5 \text{ yr})\) survive long enough to get to change the composition of future rocky cores. For example, in our models, the gaseous CO abundance in the midplane at the center of the gap is of the order of \(10^{-6}\). If the mass flow is of the order of \(10 M_\oplus\) Myr\(^{-1}\), the gaseous CO mass flow is \(10^{-5} M_\oplus\) Myr\(^{-1}\), which could be higher inside the CO snow line. When the CO reaches the border of the gaps to colder regions, it can be adsorbed by dust grains or freeze-out in cold regions of the midplane.

**Figure 16.** Radial and meridional mass flows azimuthally integrated for a 3D hydrodynamical simulation with a 0.09 Jupiter mass planet embedded at 100 au and \(\alpha = 10^{-5}\). Even for a small giant planet, the circulation around the planet’s location in the midplane reaches values higher than \(10 M_\oplus\) Myr \(^{-1}\) in the radial direction. The meridional mass flow is also large enough to exchange the chemical species from upper layers in the disk atmosphere with the midplane of the disk. The gaseous species relatively more abundant in the gap can get carried toward the gap edges and dust-rich zones, enriching dust grains and future rocky seeds.
Besides radial flows, there is also meridional circulation. The vertical velocity in the middle of the gap would be of the order of $0.1c_s$, with $c_s$ the local sound speed (Fung & Chiang 2016). Assuming that velocity, the meridional flow timescale is $\tau_{\text{mf}} = H/0.1c_s = 10/\Omega \approx \tau_{\text{orbit}}$. At 100 au, the orbital timescale for our stellar parameters is $\tau_{\text{orbit}} \approx 1000$ yr. Under a timescale of 1000 yr, the species at different substructures of the disk can be carried from one to the other, effectively enriching regions where otherwise they would not be present.

It is noteworthy that the parameters of the hydrodynamical simulation used a low viscosity value with a planet mass of roughly 0.09 Jupiter masses. A more massive planet and a higher viscosity would only increase the mass flow and shorten the timescales for the circulation. With shorter circulation timescales, the chemical equilibrium and chemical enrichment will probably differ.

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