Ice lines and disk structure in protoplanetary disks: a chemistry time-dependent approach\textsuperscript{a}

\textit{In preparation}

Abstract

Planet formation and composition is strongly connected with the composition of ice, with the position of the ice lines and their formation time within the disk evolution. The timescale of the chemistry in the ice regions is comparable to a significant fraction of the disk lifetime, making the evolution of these regions a complex interplay between evaporation, freeze-out and disk structure evolution. We explore here in a time-dependent chemistry approach, the evolution of the structure of the ice reservoirs of H\textsubscript{2}O, CO, NH\textsubscript{3}, CO\textsubscript{2} and CH\textsubscript{4} for a set of three parameters affecting continuum opacity (dust-to-gas mass ratio, maximum dust size, dust size power law distribution index), and three affecting the thermal desorption of ices (cosmic rays ionization rate, chemical efficiency heating, radioactive decay of nuclides). We model the change in ice lines as a function of time. Our numerical tests are performed with parametrized disk models computed with the radiation thermo-chemical code ProDiMo. For each model, we compute time-dependent chemistry, conserving all other disk properties. We test a simplified prescription for the ice reservoirs extent based on equilibrium between adsorption and desorption processes. To demonstrate the impact of changing ice reservoirs, we studied its effect on the CO isotopologues in gas mass diagnostics and ALMA channel maps. Limitatively to the pure adsorption/desorption processes and neglecting a full surface chemistry approach, the extent of the ice reservoirs is unaffected by the evolution of the chemistry beyond about 5\times10^{5} yrs. The only cases, in which we found a relevant change, is for
optically thin models, like the ones with flat dust size power law distribution or large maximum dust size. In those cases, the outer disk ice reservoir gets more extended radially with time. The simplified approach allows models without a chemical network to estimate quite accurately ice lines of several species. Given an integration time of 48 hrs, the noise in the ALMA line cubes is small enough that we see a hint for the presence of the rear side of the pattern in the channels maps in a disk around a typical T Tauri. However, we found different lengths of the channels maps branches (hereafter butterflies) for the different isotopologues lines in the disk models. Time-dependent chemical effects of pure gas phase network without full surface chemistry, are not a relevant factor in the spatial extent of the ice lines in protoplanetary disks in star forming regions of 1-3 Myrs, making simplified approaches as the chemical equilibrium relation a valid method for computing the size of the different ice reservoirs. Models that are optically thicker in the continuum, will have both vertically and radially more extended ices reservoirs, while the parameters affecting thermal desorption will affect the extent only in the case of very high cosmic rays ionization rate (> $10^{-12}$ s$^{-1}$), where the ice reservoirs are less extended. The gas column densities in the models with more extended ices are also lower and the line fluxes weaker. Uncertainties in models including surface chemistry and with different initial conditions, will play a role in the spatial extent of the ice reservoirs and the composition, in particular at epochs earlier than 1000 yrs. Information retrieved from CO isotopologue line ratios suffers from strong degeneracy with several disk properties, and can be used as a method for disk gas mass estimation only within a factor 10. We developed a method to measure the length of the butterflies and we found that it can partially break the degeneracy.

5.1 Introduction

H$_2$O is one of the most abundant volatiles in disks, and it is considered important also for the planet formation procedure and composition, since the ices increase the surface density of solids, and in the ice regions of the disk, the relative abundance of water is comparable to silicates and iron (Pollack et al. 1994). The inner edge of the region in the disk in which water freezes is called “snow line”. Its position depends on the gas pressure, the temperature range in which water can freeze in disks (between 145 K; Podolak & Zucker 2004; and 170 K Sasselov & Lecar 2000).

Several works on the Solar nebula investigate the position of the snow line and migration during the disk lifetime. Sasselov & Lecar (2000) modeled a passive/active flared disk irradiated by a 0.5 M$_\odot$ central star, finding that the snow line position should be within 3 au, and in the passively irradiated case it can be extended inward till 0.7 au. Podolak & Zucker (2004) state that the snow line is always located in regions where $T_{\text{dust}} \leq 150$ K, since in these regions the
5.1 Introduction

disk is optically thick, and not affected by photodesorption. Leccar et al. (2006) pointed out the role of viscous heating and disk surface density for setting the position of the snow line. Even a typical T Tauri disk accretion rate \(10^{-8} \text{M}_\odot/\text{yr}\) would be able to move outward the ice reservoir to 1.6-1.8 au. Contrary to previous studies, Garaud & Lin (2007) found that below an accretion rate of \(10^{-9} \text{M}_\odot/\text{yr}\), the snow line migrates again outward, due to the fact that passive disks are more flared, and so intercept more radiation. They even found that the snow line should migrate back inward after intense accretion events (FU Ori outburst like) on a century timescale. Martin & Livio (2012) modeled the snow line in a protoplanetary disk around a T Tauri star. They found that in the presence of a “Dead zone”, the inner edge of the ice reservoir cannot be closer than 3.1 au.

Modeling disks with dust grains larger than the typical ISM dust grain size, Mulders et al. (2015) found that the location of the snow line should be inward by a factor two with respect previous predictions of 2-5 au. They also found that assuming ISM-type dust, the position of the snow line would make inner planets dry around low mass PMSs \((M_\star < 0.5 \text{M}_\odot)\).

In the disk lifetime processes like molecular diffusion and mass transportation of ice covered dust grains play an important role in the disk ice reservoirs structure: diffusion processes are able to increase the outer disk ice mass, due to cyclical events of freezing and mass transportation of dust grains in the outer disk, enhancing giant planet formation (Zhang & Jin 2015). The evaporation process in the inner disk is responsible for cooling processes that promote instabilities and pressure inversions able to stop planetesimals migration (Wang 2015).

CO is also another abundant volatile \((\sim 10^{-4} \text{ relative to H}_2; \text{ Liu et al. 2013})\). The “ice line” of CO is further out compared to water, and this creates an additional solid mass repository in the outer disk, where giant planets are formed. Recently CO ice line have been indirectly observed in TW Hya, through N\(_2\)H\(^+\) ALMA observations (Qi et al. 2013). Mathews et al. (2013) used instead DCO\(^+\) as a probe to image the CO ice line around HD 163296, finding a location consistent with the typical 19-20 K freeze-out temperature. The constrain of the CO ice line conditions for HD 163296 is confirmed by de Gregorio-Monsalvo et al. (2013), using CO and isotopologues ALMA detections. ALMA observations of DCO\(^+\) towards IM Lupi show a two ring structure in the disk, the internal one \((\sim 25 \text{ au})\) consistent with the CO thermal ice line, and the external one \((\sim 200 \text{ au})\) is consistent with non-thermal desorption of CO from the ice reservoir Öberg et al. (2015a).

The NH\(_3\) ice line is almost co-spatial with water, and it contributes up to the 7% in mass to the inner ice reservoir (Dodson-Robinson et al. 2009). Finally CH\(_4\) is another volatile that adds mass to the outer ice reservoir.

Previous works focused on the effects of disk instabilities, structure and heating/cooling (including accretion) on ice reservoirs, and in particular focused on the snow line. Here we treat for the first time in 2D with a full radiation thermo-
5.2 Modeling

We describe in this section the code ProDiMo and the series of models we developed to study which properties affect the ice line of five main volatiles in disks (H$_2$O, CO, CO$_2$, CH$_4$, NH$_3$). In a second subsection, we treat a simplified approach to define the ice lines without a complete chemical computation.

5.2.1 Parameter space of models

We model the snow line, and the CO, CO$_2$, CH$_4$ and NH$_3$ ice lines computing a series of time dependent disks models using the radiation thermo-chemical code ProDiMo (“Protoplanetary Disk Model”) including X-ray photoprocesses (Woitke et al. 2009a, Aresu et al. 2011), adopting the same method used in a previous study by Meijerink et al. (2013) towards AGNs dust tori. In this mode the code integrates for the required time the chemical rate equations, solving the heating/cooling balance at every step. The chemical network rates are taken from UMIST 2012 (McElroy et al. 2013) for a gas phase network of 100 species. Heating processes implemented include PAH/photoelectric heating (Bakes & Tielens 1994), C photoionization, H$_2$ photodissociation, formation heating and collisional de-excitation, cosmic ray heating, chemical heating, and viscous heating. Cooling processes include Ly-$\alpha$, OI 630 nm, and more than 10000 atomic/molecular emission lines from 89 gas species. Gas and dust thermalization is also taken into account. In addition, photo-rates are computed using detailed cross-sections and the local radiation field in the disk. We use a tapered-edge description of the outer disk. Additional processes described in Woitke et al. (2011) include the PAH ionization balance, UV fluorescence pumping, a parametric description of settling, pumping by OH photodissocation, H$_2$ pumping by formation on dust grains.

We run several series of models exploring different values for six parameters (Table 5.1). The first three are related to continuum opacity and dust properties (dust-to-gas mass ratio, dust maximum size, dust size power law distribution index). The second three parameters produce effects on the chemistry, ionization degree, and heating in the embedded regions of the disk (chemical efficiency heating, cosmic rays ionization rate, ionization rate from radioactive nuclei). Chemical efficiency is the fraction (spanning from 0 to 1) of energy produced by exothermic reactions that we decide to put into gas kinetic energy, and not
distributed into other degrees of freedom of the reaction products. Radioactive decay heating is attributed specifically to some nuclides that contributes relevantly in the environment of a young star. The largest contribution is due to $^{26}\text{Al}$, which ionization rate is $7.3 \times 10^{-19}$ s$^{-1}$ and is a short life radionuclide. Considering long live radionuclides, the global ionization rate would be driven by $^{40}\text{K}$ and other nuclides as $^{235,238}\text{U}$, and the total ionization rate due to these nuclides is $1.4 \times 10^{-22}$ s$^{-1}$ (Umebayashi & Nakano 2009). We model cases of very high cosmic rays ionization rate, considering that the astroparticle flux is stronger in environments with particularly strong Star Formation Rate (like starburst galaxies) and or AGNs. Even in our Galaxy there are clues about an enhanced flux in diffuse clouds and in Orion Bar (Gupta et al. 2010, Neufeld et al. 2010). The highest ionization rate here considered is from models of cosmic rays dominated regions (CRDRs; Bayet et al. 2011).

Each model is a time dependent run through five epochs spanning from the early disk phase up to the typical disk lifetime of 5 Myrs (Table 5.2). The structure and properties of our standard disk model are described in detail in Appendix A.1.

### 5.2.2 A simplified approach for ice lines in disks

We present here an approach to describe the ice reservoir extent based on the sublimation equilibrium relation between ices and gas in the disk. This equilibrium is described by the adsorption process, and the thermal and non-thermal desorption processes. The adsorption rate depends on the gas temperature $T_{\text{gas}}$ [K], molecular mass of the species $m_{\text{molec}}$ [g], dust density $n_{\text{dust}}$ [cm$^{-3}$], and average dust grain size $\langle a \rangle$ [cm] defined accordingly to Woitke et al. (2009a)

$$R_{\text{ads}} = 4\pi\langle a \rangle^2 n_{\text{dust}} \alpha \sqrt{\frac{k_b T_{\text{gas}}}{2\pi m_{\text{molec}}}} \quad [\text{s}^{-1}] \quad (5.1)$$

The sticking coefficient $\alpha$ is set to 1 in all the species heavier than He in our computation (according to; Burke & Hollenbach 1983). The thermal desorption rate is given by

$$R_{\text{Th-des}} = \sqrt{\frac{2n_{\text{surf}} k_b E_{\text{ads}}}{m_{\text{molec}} \langle a \rangle^2}} e^{-\frac{E_{\text{ads}}}{k_b T_{\text{dust}}}} \quad [\text{s}^{-1}] \quad (5.2)$$

This process depends on the surface density of binding sites on the dust grains $n_{\text{surf}}$ [cm$^{-2}$], the adsorption energy on dust grains $E_{\text{ads}}$ [K] of the molecule considered, the dust temperature $T_{\text{dust}}$ [K], and again the molecular mass [g]. $k_b$ is the Boltzmann constant [g cm$^2$ s$^{-2}$ K$^{-1}$].

The non-thermal process of desorption we consider is photodesorption
### Chapter 5 – Ice lines and disk structure in protoplanetary disks

**Table 5.1 – Standard disk and parameter space**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photospheric temperature</td>
<td>$T_{\text{eff}}$ [K] 4400</td>
<td></td>
</tr>
<tr>
<td>Stellar mass</td>
<td>$M_*$ [M$_\odot$] 0.8</td>
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</tr>
<tr>
<td>Stellar luminosity</td>
<td>$L_*$ [L$_\odot$] 0.7</td>
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<tr>
<td>FUV excess(*)</td>
<td>$L_{\text{UV}} / L_*$ 0.01</td>
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<td>UV power law exponent</td>
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<tr>
<td>X-ray luminosity</td>
<td>$L_X$ [erg/s] $10^{30}$</td>
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</tr>
<tr>
<td>X-ray minimum energy</td>
<td>$E_{\text{min},X}$ [keV] 0.1</td>
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</tr>
<tr>
<td>X-ray Temperature</td>
<td>$T_X$ [K] $10^7$</td>
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</table>

**Standard disk model parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid points</td>
<td>$N_{xx}/N_{zz}$</td>
<td>$70 \times 70$</td>
</tr>
<tr>
<td>Disk gas mass</td>
<td>$M_{\text{gas}}$ [M$_\odot$] 0.01</td>
<td></td>
</tr>
<tr>
<td>Inner radius</td>
<td>$R_{\text{in}}$ [au] 0.1</td>
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<tr>
<td>Outer radius</td>
<td>$R_{\text{out}}$ [au] 300</td>
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</tr>
<tr>
<td>Surface density power law index</td>
<td>$\epsilon$</td>
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<tr>
<td>Minimum dust size</td>
<td>$a_{\text{min}}$ [$\mu$m] 0.05</td>
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<tr>
<td>Tapering-off radius</td>
<td>$R_{\text{taper}}$ [au] 200</td>
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<tr>
<td>Settling description</td>
<td>-</td>
<td>Dubrulle</td>
</tr>
<tr>
<td>Turbulent mixing parameter</td>
<td>$\alpha$</td>
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<tr>
<td>distance</td>
<td>$d$ [pc]</td>
<td>140</td>
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<tr>
<td>Turbulence viscosity coeff-</td>
<td>$\alpha_{\text{vis}}$ [-] 0</td>
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</tr>
</tbody>
</table>

(*) The presence of UV excess is not consistent with the disk accretion. The disks are all passively heated.

**Table 5.2 – Disk parameters explored**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Grid values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dust-to-gas mass ratio</td>
<td>$d/g$</td>
<td>0.001, 0.01, 0.1, 1, 10, 100</td>
</tr>
<tr>
<td>Dust power law index</td>
<td>$a_{\text{pow}}$</td>
<td>2.0, 2.5, 3.0, 3.5, 4.0, 4.5</td>
</tr>
<tr>
<td>Dust maximum size</td>
<td>$a_{\text{max}}$ [$\mu$m] 250, 400, 500, 700, 1000, 2000, 5000, $10^4$, $10^5$</td>
<td></td>
</tr>
<tr>
<td>Chemical efficiency heating</td>
<td>-</td>
<td>0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0</td>
</tr>
<tr>
<td>Cosmic ray ionization rate</td>
<td>$\zeta_{\text{CR}}$ [s$^{-1}$] 1.7 (−19), 1.7 (−18), 1.7 (−17), 1.7 (−16), 1.7 (−15), 1.7 (−14), 1.7 (−13), 1.7 (−12)</td>
<td></td>
</tr>
<tr>
<td>Radioactive decay ionization rate</td>
<td>$\zeta_{\text{Rad}}$ [s$^{-1}$] 0.0, 1.4(−22), 7.3(−19)</td>
<td></td>
</tr>
<tr>
<td>Disk ages</td>
<td>$t$ [yr]</td>
<td>$10^3$, $5\times10^3$, $10^4$, 2.5$\times10^5$, 5$\times10^6$</td>
</tr>
</tbody>
</table>

(*) The presence of UV excess is not consistent with the disk accretion. Our disks are all passively heated. Bracket notation $x(y)$ means $x \cdot 10^y$. 

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5.3 Results

\[ R_{\text{Ph-des}} = \pi \langle a \rangle^2 \frac{n_{\text{dust}}}{n_{\text{layers}}} \phi_{\text{photon}} \chi F_{\text{Draine}} \quad [\text{s}^{-1}] \]  

(5.3)

It depends on the FUV radiation field intensity (\( \chi \)) expressed in units of the Draine field \( F_{\text{Draine}} (G_0; \text{Draine 1978}) \). \( \phi_{\text{photon}} \) is the photo desorption yield. The numerical density of active ice layers on dust grains is described as

\[ n_{\text{layers}} = 4\pi \langle a \rangle^2 n_{\text{dust}} n_{\text{surf}} N_{\text{layers}} \]  

(5.4)

in which \( n_{\text{surf}} \text{[cm}^{-2}\text{]} \) is the surface density of sites. \( N_{\text{layers}} \) is the number of active layers. In our modeling we consider 2. The last non-thermal desorption process included in our treatment is induced by cosmic-rays

\[ R_{\text{CR-des}} = 3.16 \cdot 10^{-19} \frac{\zeta_{\text{CR}}}{5 \cdot 10^{-17} \text{s}^{-1}} R_{\text{Th-des}}(70 \text{ K}) \quad [\text{s}^{-1}] \]  

(5.5)

Here, \( \zeta_{\text{CR}} \text{[s}^{-1}\text{]} \) is the cosmic ray ionization rate, and the process is based on a thermal cycle, in which the dust grain is locally heated (thermal spike) and then cooling timescale is taken into account. This process is dependent from the assumptions on dust grains specific heat and temperature (Hasegawa & Herbst 1993).

We define the ice line as the location where the abundance of gas and ice are equal. Then the position of this transition becomes simply the place in the disk where the above described four rates are in balance and the densities of both ice and molecules in the gas are equal.

\[ R_{\text{ads}} = R_{\text{Th-des}} + R_{\text{Ph-des}} + R_{\text{CR-des}} \]  

(5.6)

This allows us to compute its position without taking the full gas chemistry into account, only knowing the radiation field, the dust temperature and the cosmic rays flux. In the following, we will check this simplified approach against detailed thermochemical models.

5.3 Results

Here we discuss our results on the timescale on which ice reservoirs change in disks with different properties. We also test the sensitivity of our results to the initial conditions (abundances), how much the surface chemistry will affect the spatial extent of the ice lines, and the reliability of our simplified disk reservoir prescription.
5.3.1 Time evolution of ice reservoirs in disks

The aim of this study is to find out whether the spatial extent of the ice reservoirs change over the typical lifetime of a disk. We base the outline of the ice reservoir on an abundance criterium \( n_{\text{gas}} = n_{\text{ice}} \) and draw the contours of the ice reservoirs retrieved at the different epochs. In our standard disk model (Fig. 5.3.1), the ice reservoirs are not changing with time beyond 0.1 Myrs. The extent of the reservoir is marginally affected only in the outer disk, that is bolometrically optically thin, and has a longer timescale for the chemistry. However, we generally computed from this epoch because on average we observe protoplanetary disks with ages around \( 0.1-10^6 \) yrs, and we wanted to analyze if at this stage ice reservoirs are expected to change with a chemistry time-dependent approach.

Figure 5.1 – Standard disk model. The black line delimitate the disk region with \( n_{\text{gas}} \geq 3000 \) cm\(^{-3}\). The different linestyle is used to trace the different ices reservoirs: thick for water, dotted for CO, dashed for CO\(_2\), dot-dashed for CH\(_4\), “x” for NH\(_3\). The color of each contour is coded for the epoch at which it is defined. The actual position of Earth and Jupiter in the Solar System is reported by the respective symbols.
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Our modeling approach is affected by assumptions and uncertainties: 1) our initial conditions of the time-dependent computation are based on molecular cloud initial abundances obtained from a steady-state chemical modeling, 2) our network consists of gas phase reactions and adsorption/desorption processes, and is largely based on UMIST 2012.

Considering shorter timescales, ice reservoirs expand outward and upward with time in the disk regions beyond 3-4 au of our standard model. This happens in the first $10^5$ yr (Fig. 5.3.1). The reason for this radial expansion of the ice reservoirs is a consequence of the rich presence of volatiles in gas phase, out of equilibrium with the ice, and that freeze on dust with a relatively slow timescale.

![Figure 5.2](image)

**Figure 5.2** – Contours of the ice reservoirs in our standard model including epochs earlier than $10^5$ yr.

5.3.2 Effects of dust opacity on ice reservoirs

The extent of the ice reservoirs depends particularly on the disk dust opacity (Fig. 5.3). In the models with higher continuum opacity (high $d/g$, low $a_{pow}$,
low $a_{\text{max}}$), the reservoirs are more extended both inward and vertically, for two reasons. The gas in the disk is colder, since the radial temperature gradient becomes steeper (because radiation penetrate less). Also photodesorption is reduced in the outer disks, where FUV photons cannot penetrate anymore. The ice reservoirs extent in most cases does not change with time. Only for a very flat dust size power law distribution, we find that the ice lines become more extended in the outer disk between 0.1 and 5 Myrs. Different parameters produce also similar effects on the ice reservoirs extent in disks. Disks with very low dust content (Fig. 5.3 c) produce a spatial extent of the ice reservoirs identical to that produced by a very large maximum dust size (Fig. 5.3 f). Then disks with very steep dust size power law distribution (Fig. 5.3 b) will have similar ice reservoirs extent than disks with very high dust content (Fig. 5.3 d). These two models will have a very reduced volatiles gas column densities, in particular beyond 1 au.

5.3.3 Effects of chemical heating and ionization rate on ice reservoirs

The second series of parameters we modeled, chemical heating, cosmic-ray and radioactive nuclei ionization rate, affect properties like gas heating and/or ionization degree. Only the cosmic rays (Fig. 5.4 d) shrink the size of the ice reservoirs in disks, producing therefore a larger gas column density in the outer disk, but here we are considering an extremely (and probably unrealistic) ionization rate. Radioactive decay of nuclei has a contribution to ionization that is up to two dex less than cosmic rays for the same model, the consequent heating is also marginal, and the ice reservoirs are unaffected (Fig. 5.4 f). The chemical heating is dominant in the warm surface gas layers, and is negligible in the cold regions of the disk, where ice forms (Fig. 5.4 b). Also this parameter does not affect the ice reservoirs extent.

5.3.4 Approximate ice line definition

A computationally very expensive part of our and several other codes, is the chemistry solver. Given a thermo-physical solution for the dust, i.e. knowing $T_{\text{gas}}$ and $T_{\text{dust}}$, and the local FUV radiation field, it is possible to compute the spatial extent of the ice reservoirs in an approximate way. This approach excludes the need for the full chemical treatment, and allows a simple prescription for the ice spatial extents that can be potentially used in non-chemical codes (see

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1 These two temperatures can be considered equal in the optically thick regions of the disk, and this assumption holds also in large parts of the the optically thinner regions of the outer disk, where the ices reside.
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Figure 5.3 – Contours of the ice reservoirs time variation for the models with different dust opacity; plots are shown only for the extremes of the explored parameter range. (a) $\alpha_{\text{pow}} = 2.0$, (b) $\alpha_{\text{pow}} = 4.5$, (c) $d/g = 0.001$, (d) $d/g = 100$, (e) $a_{\text{max}} = 250 \ \mu m$, (f) $a_{\text{max}} = 10 \ \text{cm}$. For details about the plots check the caption of Fig. 5.3.1.
Figure 5.4 – Contours of the ice reservoirs time variation for the models with different heating/ionization rate, plots for the extremes of the explored dynamic range. (a) chemical efficiency heating 0%, (b) chemical efficiency heating 100%, (c) $\zeta_{\text{CR}} = 1.7 \cdot 10^{-19} \text{ s}^{-1}$, (d) $\zeta_{\text{CR}} = 1.7 \cdot 10^{-12} \text{ s}^{-1}$, (e) $\zeta_{\text{radioactive}} = 0.0 \text{ s}^{-1}$, (f) $\zeta_{\text{radioactive}} = 7.3 \cdot 10^{-19} \text{ s}^{-1}$. For details about the plots check the caption of Fig. 5.3.1.
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Our method based on the rate equilibrium, is the only one that is completely independent from the gas physical and chemical properties, and can be directly appliable to pure continuum radiative transfer codes.

The criterium based on the rate balance produces an approximate description of the real extent of the reservoirs for H$_2$O, CO, NH$_3$. The ice line of CO$_2$ and CH$_4$ are less accurately described in their spatial extent (Fig 5.5). The main reason for the discrepancies is a simplified definition of the local radiation field.

In Min et al. submitted, the water snow line is defined through a density criterium. For our scope, we adapted the criterium defining the vapor pressure of the ice and comparing it directly with the local partial pressure of the molecular gas in question

$$P_{\text{vap}}(\text{H}_2\text{O}) = \frac{k_B T_{\text{gas}}}{m_{\text{H}_2\text{O}}} \left( \frac{10^{B-A/T_{\text{gas}}}}{T_{\text{gas}}} + \gamma \frac{G_{\text{UV}}}{\sqrt{T_{\text{gas}}}} \right)$$

(5.7)

The first term in parenthesis is a purely thermodynamic term from the equilibrium between the phases, the second is a corrective factor that takes into account photodesorption. This pressure is a function of the gas temperature $T_{\text{gas}}$, the molecular mass of the species (water in that case, $m_{\text{H}_2\text{O}}$), the local FUV radiation field computed from the radiative transfer in Draine units $G_{\text{UV}}$, the Boltzmann constant $k_B$, and two coefficients that account for the phase transition enthalpy $A, B$. Finally the scaling parameter $\gamma$ is set to $10^{-20}$ to give good agreement with the detailed ProDiMo calculations, and is the same for all the species. We adopted the previous definition for CO, applying proper coefficients $A$ and $B$ in order to delimitate the corresponding ice line. In Williams & Best (2014), the CO ice line is defined in the region of the disk where $T_{\text{gas}} = 20$ K and $N_{\text{H}} > 1.3 \cdot 10^{32}$ g/cm$^{-2}$, the column density above which photodesorption effects are negligible. Using the three previous criteria, we also computed the gas column densities, adopting a numerical procedure described in Appendix A.2.

The results of the three criteria are compared in Fig. 5.6. The agreement in outlining the CO ice reservoir is reasonable for Williams & Best (2014) and our rate method, while Min et al. method deviates significantly. The difference is mainly reflected in the outer disk: The Min et al. criterium yields two dex less CO column density and a final mass that is $\sim 40\%$ less than the other three definitions. This difference is due to the bad definition of the CO ice line beyond 50 au (Fig. 5.6). The difference from Williams & Best (2014) and our rate methods (that are in strong agreement) is about $5\%$ in mass (beyond 10 au).

In the case of water, the outlining of the ice reservoir based on the rate criterium is less accurate than for the case of CO. Our definition of the ice reservoir underestimate by two dex the column of water vapor in the outer disk (Fig. 5.7). The criterium adopted by Min et al. for water produce a comparable mismatch in terms of column density definition. All the three method differ between each other of a dex in terms of ice mass beyond 0.9 au, with Min et al. predicting two dex less gas mass than the ProDiMo computation. The
Figure 5.5 – Ice relative abundances and ice line computed from detailed balance between desorption and adsorption processes, compared with a simple $T_{\text{dust}}$ criterion. For each species, the freeze-out temperatures have been taken from Table 1 of Bockele-Morvan (1997) (except for NH$_3$, that is assumed to sublimate at a temperature similar to water). Water ice (top left), CO ice (top right), CO$_2$ ice (middle left), CH$_4$ (middle right), NH$_3$ (bottom).
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Figure 5.6 – CO ice line and gas column density. Left: Comparison of the different methods to define the CO ice line; rate based method (blue), critical pressure criterium discussed in Min et al. submitted (white), criterium used in Williams & Best (2014) (black). Right, gas column density applying the three ice line definitions, the orange thick line shows the outcome from ProDiMo, and computed CO gas masses beyond 10 au.

Figure 5.7 – H2O ice line and gas column density. Left: Comparison of the different methods to define the snow line; rate based method (blue), critical pressure criterium discussed in Min et al. (yellow). Right: Gas column density applying the two ice line definitions previously discussed and computed water gas masses beyond 0.9 au.
main effect of these differences is reflected in the spectroscopy. If the gas column density is underestimated by two orders of magnitude in this disk region, far-IR lines (like the ones observed by Herschel PACS) can be heavily underpredicted. In addition, the far-IR ice features produced from these regions of the disk would be overpredicted (because of larger ice column densities), and expected to be produced from higher surface layers.

5.3.5 Sensitivity to the initial conditions

The time dependent simulations we performed in this work are based on molecular cloud initial abundances. In the cold and most embedded regions of protoplanetary disks, the timescales of the chemistry are very long and comparable with the disk lifetime. Differences in the initial abundances can affect the chemical abundances at all timesteps. To test this, we decided to run single point chemistry models for the physical conditions of two points close to the water ice reservoir (Table 5.3) in time-dependent chemistry mode. We consider more than 230 epochs spanning 1 to $10^8$ yrs. Over this timescale the final abundances, also of the regions of the disks affected by the slowest chemistry, should be converged to steady state abundances (Fig. 5.8).

Our typical starting conditions for the time-dependent chemistry consider the abundances from molecular clouds, obtained through a steady-state solution for the physical conditions: density, gas and dust temperatures, extinction, radiation field (values are reported in Table 5.4), and initial gas composition from UMIST molecular cloud abundances. In our test, we exchange ice abundances with the correspondent gas ones for the species that have ices included in the chemical network (Table 5.5). With our simplified ice network, the main processes involving ices are adsorption/desorption, considering that these reactions have very long timescales, an upsetting of the initial abundances represent
Figure 5.8 – Single grid point time-dependent tests. Top plots are for standard abundances (left) and inverted abundances (right) at 1 au (z = 0.12 au). Bottom plots are the same but for 10 au (z = 8 au). Continuous lines are for the gas phase species, dotted lines are for the ices. Legend of all the figures is plotted only on the bottom right plot for convenience.
an extreme test about the sensitivity to the initial conditions. These different initial abundances produce effects on the gas composition within the first $10^7$ yrs in the inner disk. This is a timescale consistent with the expected disk lifetime (e.g. Haisch et al. 2001, Yasui et al. 2012), and even beyond $10^7$ yrs for the outer disk. Hence, any discussion based on time-dependent chemistry in disks is strongly dependent on the assumed initial abundances.

We tested the sensitivity of the ice reservoir time evolution for different initial conditions, adopting an initial set of abundances recommended from UMIST 2012 (McElroy et al. 2013). From the full 2D test (Fig. 5.9), we found that time evolution still happens within $10^5$ yr and the vertical and radial extent in time evolve similarly as for the case of our standard abundances. The main difference is in the vertical extent of the ice reservoirs of water, that at 0.3-1 au is below $z/r = 0.2$, and CO$_2$ that is initially very vertically extended, above $z/r = 0.2$. However, from single grid point chemistry, we found that different initial abundances produce a different time evolution in the composition of ices and gas (Fig. 5.8 & 5.12). This means that the mass of individual ice species is changed but the ice lines are less affected.

Figure 5.9 – Contours of the ice reservoirs in our standard model with the abundances recommended from UMIST 2012 (McElroy et al. 2013).
5.3.6 Surface chemistry

Surface chemistry is thought to play an important role in setting the ice abundances. However, the microscopic processes leading to the formation of ices are still under investigation and different network produce different results. Behind the uncertainties there are different methods for computing the surface chemistry: Rate equation (e.g. Cuppen & Garrod 2011), Monte Carlo simulations (e.g. Caselli et al. 2002, Cazaux et al. 2010), Master equation method (e.g. Stantcheva et al. 2002, Garrod et al. 2009). Besides the different methods, there are uncertainties in the physics itself, related with the barrier and binding energies. For example, the reaction $\text{H} + \text{CO}$ is assumed to have a barrier of $\sim 2000$ K in Garrod et al. (2007), while Fuchs et al. (2009) computed an activation energy of $\sim 400$ K for the same reaction. An additional complication is the multi-layer aspect of ice, produced by the formation of iced mantles on the dust grain with a complex structure (Taquet et al. 2012). In the following we approach the surface chemistry through a series of steps with increasing complexity.

5.3.6.1 Surface chemistry of water

Several studies have been performed for water formation on dust grains. It is widely accepted that this is an alternative way to produce this molecule in dark molecular clouds (e.g. Lamberts et al. 2014). The accepted water formation mechanism on ice has been theorized from Tielens & Hagen (1982), and then tested in lab experiments. It can be branched in three main channels (van Dishoeck et al. 2014), plus a fourth that uses the direct reaction of $\text{H}_2$ and OH on dust grains, that is a very efficient water surface chemistry formation channel in translucent clouds (Cazaux et al. 2010). All of them except the fourth start with the adsorption of atomic oxygen on dust grains. Due to the larger abundance of H and $\text{H}_2$, the limiting reactant in this process will be always O. Hence its abundance will determine how much water can be produced onto dust grains.

The only mechanism for water formation we consider here is an Elay-Rideal process. This process happens in warm regions of the interstellar medium and protoplanetary disks, where the lifetime of ices is very short (He & Vidali 2014), however, we found that it does not affect the snow line (Fig. 5.10).

The distribution of O ice is within the water ice reservoir in the outer region of the disk. This means that any surface chemistry would affect only the total mass of ices and not the spatial extent of the snow line (Fig. 5.10).
Figure 5.10 – Ice relative abundance in the standard disk model for the steady state solution. Water ice line is compared with Oxygen ice line, based on the abundance criterium ($n_{\text{ice}} = n_{\text{gas}}$).
5.3.6.2 Surface chemistry of carbon dioxide

Carbon dioxide can be produced through surface reactions in cold gaseous environments. Lab studies show three main processes that contributes to the formation of this molecule:

\[ \text{s-CO} + \text{s-O} \rightarrow \text{s-CO}_2 \text{ (Roser et al. 2001)} \]

\[ \text{s-CO} + \text{s-OH} \rightarrow \text{s-CO}_2 + \text{s-H} \text{ (Raut & Baragiola 2011)} \]

\[ \text{s-H}_2\text{CO} + \text{s-O} \rightarrow \text{s-CO} + \text{s-O} \text{ (Minissale et al. 2015)} \]

Considering the relative abundance of the precursor species, the main processes contributing to the solid-phase formation will be the first two. The CO ice abundance in the ice reservoir is about 2 dex larger than both O and OH ices. Reservoirs of CO and O starts beyond 9 au, with O being the less extended. OH ice reservoir extends even inward up to almost 1 au (Fig 5.11). The presence of CO and O ices in the outer disk, makes possible to increase the mass of the CO$_2$ ice reservoir in the outer disk, but not the spatial extent.

5.3.6.3 Full surface chemistry network

Our chemical network is based on a limited amount of ice species and all molecular (H$_2$O, CO, CO$_2$, CH$_4$, NH$_3$, SiO, HCN, SO$_2$, O$_2$, N$_2$), and 90 gas phase species (DIANA small standard; Kamp et al. in prep.). The effect of the surface chemistry on this limited range of species is negligible because we are not considering more complex species such as methanol (which is formed mainly through surface chemistry) and we neglect atomic ices (that are potential precursors of the molecules we are instead considering in ices). In the single point test with surface reactions (Fig. 5.12), we included also ices of Si, Mg, Fe, O, OH, C$_2$, CH$_3$OH, and the difference is clearly visible compared to the plots on the right of Fig. 5.8. A full surface chemistry network that does not includes other ice species as the atomic ones that are precursors of ice molecules, will produce the same results of a pure gas phase network. Hence the conclusion produced from the pure gas phase network with adsorption/desorption processes hold only for the simple ices we considered throughout.

The full 2D surface chemistry is computationally very expensive, also because it requires an extended network (239 species) including several atomic ices. Including these reactions, the size of all the ice reservoirs is completely changed (Fig. 5.13), Water ices are vertically more extended beyond 2 au and up to the disk surface beyond 20 au. CO$_2$ and NH$_3$ shows a similar behavior. These two ice reservoirs at the first epochs are even more extended vertically.
Figure 5.11 – Ice relative abundance in the standard disk model for the steady state solution. CO$_2$ ice abundance is compared with the ice lines of Oxygen, CO, OH, based on the abundance criterium ($n_{\text{ice}} = n_{\text{gas}}$).
in the outer disk beyond 100 au, in particular water, that needs longer epochs to be depleted by photodesorption in the upper regions of the disk. The most interesting case is the CO ice reservoir; it expands strongly both radially and vertically until it reaches the outer disk and stretches up to \( z/r \sim 0.18 \). All the other ice reservoirs are already extended up to \( R_{\text{out}} \) at 100 yrs.

In these tests we adopted a surface chemistry network from Hasegawa et al. (1992) and Hasegawa & Herbst (1993). Several other models for surface chemistry are available, and can produce different results in terms of ice reservoirs spatial evolution and extent.

### 5.4 ALMA observations and gas mass estimates

The extent and shape of the ice reservoirs have an impact on the gas column density above it. Here, we investigate how the disk properties that affect the ice reservoirs extent impact the spectral CO maps obtained with ALMA.
Figure 5.13 – Contours of the ice reservoirs in our standard model with the full surface chemistry included. The ice reservoirs of water, CO$_2$ and NH$_3$ are vertically very extended, even in regions with $n_{\text{gas}} < 3000 \text{ cm}^{-1}$ (black line).
5.4 ALMA observations and gas mass estimates

5.4.1 ALMA simulations of CO observations

We simulate ALMA observations of CO, $^{13}$CO and C$^{18}$O with the CASA simulator\(^2\), using configuration 6 of Cycle 3\(^3\) and 48 hrs of total exposure. This long and unrealistic integration times has been adopted for guarantee the sufficient $S/N$ in the single channels of the data cubes of the weakest lines. We decided to model the $J = 2 - 1$ lines for compare the fluxes from different models with the results of Miotello et al. (2014), and the $J = 3 - 2$ lines for a direct comparison with the channel map patterns (hereafter called butterflies) shown in de Gregorio-Monsalvo et al. (2013). We put the T Tauri disk model at a distance of 140 pc and assume an inclination of 30°. The different CO isotopologues are considered efficient tracers of the gas mass in disks. In a recent work de Gregorio-Monsalvo et al. (2013), through CO ALMA channel maps, observed for the first time the back surface of the disk around HD 163296. Constraining the disk structure with the ALMA channel maps of CO and isotopologues, they confirmed that the CO ice line resided at 20 K.

The less abundant isotopologues have lower line fluxes, and so less bright butterflies (Fig. 5.19-5.21). The same cube for a model with very flat power-law dust size distribution, shows more intense line fluxes, due to a combination of lower continuum opacity (Fig. A.6 b) and larger gas temperature (Fig. 5.22-5.24). If we consider a disk with a relatively high dust content ($d/g = 1$; Fig. 5.25-5.27), the butterflies look very similar to the ones of our standard model. This is however not the most extreme case we modeled, but a more likely case. The case of very large dust grains (Fig. 5.28-5.30) is similar to the very flat power law dust size distribution. Interesting is the simulation of a very high cosmic-rays ionization rate (Fig. 5.31-5.33); here the butterflies look brighter compared to the standard model, due to the slightly less extended ice reservoirs (Fig. 5.4).

The plots of Fig. 5.19-5.33 show how different disk properties produce different line fluxes and brightness profiles, due to changes in the continuum optical depth (Fig. A.6) and thermal profile of the disk. Line fluxes from the different isotopologues react in a complex manner when changing disk properties in our models leading to strong degeneracies. ALMA noise and resolution, with the given observation setup, suppress the visibility of back surface of the disk models. This will make it hard, with the specific antenna configuration and resolution chosen here, to directly locate the CO ice line in a typical T Tauri disk, similar to what was done by de Gregorio-Monsalvo et al. (2013).

To quantify changes in the butterflies, we measure the length of the butterflies in the ALMA cubes of different isotopologues through a procedure described in Appendix A.3. We picked the 0.79 km/s channel for some of the most extreme cases of the parameters we modeled. In the standard model, the

\(^2\) http://casa.nrao.edu/

\(^3\) Baseline: min 77.3 m, max 2299.6 m; 36 12 m and 10 7 m antennas. Beamsize: 0.3″(Band 3), ∼ 21 au at 140 pc.
butterflies extent is directly related to the relative abundances of the isotopologues. This is not true for models with other properties. In the case of a very flat power law dust size distribution the trend is inverted. In models with strong continuum optical depth, the length of the wings is the same for all the isotopologues. Every parameter produces its own signature in the butterflies (Fig. 5.14).

![Figure 5.14](image)

**Figure 5.14** – Length of the ALMA butterflies for the channel +0.79 km/s, considering the transition $J = 3 - 2$ for some of the models described in Table 5.2, for the three isotopologues of CO: $^{12}$CO (blue dots), $^{13}$CO (red triangles), C$^{18}$O (green squares).

### 5.4.2 CO and isotopologues as disk gas mass estimator

Williams & Best (2014) proposed the use of line ratios of the $J = 2 - 1$ transitions of $^{13}$CO and C$^{18}$O as a direct probe of the disk gas mass. We compare CO isotopologues rotational line prediction from some models of our series presented in Antonellini et al. (2015b) with the observations reported in Table 1 & 4 of Williams & Best (2014), converting their flux according to
5.5 Conclusions

\[ I_{13\text{CO},18\text{O}} = F_{13\text{CO},18\text{O}} \cdot 4\pi d^2 \quad [\text{Jy km s}^{-1} \text{ pc}^2] \] (5.8)

Here, \( d \) is the distance in pc. Errors are assumed to be 20% for each data point.

Our models show that this method is more degenerate than previously thought. Line flux ratios are shown in Fig. 5.15 for some of our models; all of them (except the ones with explicitly different \( M_{\text{gas}} \)) have a gas mass of 0.01 \( M_\odot \). The parameters studied in this paper (Table 5.2) can produce the same signature as different disk gas masses, for example a model with \( d/g = 1 \) can produce a line ratio similar to one with \( M_{\text{gas}} = 10^{-4} M_\odot \). On the other side, models with very large dust grains (\( a_{\text{max}} \) up to 10 cm or very flat power law \( a_{\text{pow}} = 2.0 \)) produce line ratios similar to the ones of a model with \( M_{\text{gas}} = 0.1 M_\odot \). In the absence of knowing detailed dust properties, this limits the accuracy of the gas mass estimate to 1 dex. The modeling results from Miotello et al. (2014), based on the \( J=3\rightarrow2 \) rotational transition, show that isotopologue selective photodissociation affects mainly the \( \text{C}^{18}\text{O} \) line flux, and only in case of very low disk mass; this is due to line optical depth effects, although the assumption of a fixed isotopologues abundance the disk structure, could produce an underestimate throughout of about 1 dex in the disk masses (Miotello et al. 2014).

5.5 Conclusions

The results of this study, based on a pure gas phase network including only adsorption/desorption processes, suggest that the role of chemistry is marginal in the definition of the spatial extent of the ice reservoirs for epochs beyond \( 10^5 \) yr. The exception are some extreme cases with unusual dust properties (very flat dust size power law distribution). Different disk properties affecting the dust size or relative content with respect to the gas will produce different extent in the ice reservoirs. In continuum optically thicker models, the ice reservoirs will be radially and vertically more extended. On the other side, the parameters affecting to heating/cooling that we considered affect only marginally the shape of the ice lines. Only an extremely high cosmic ray flux will modify the outer shape of the ice lines.

The limitation due to the initial conditions we considered for our time-dependent integration (molecular cloud abundances), will affect partially the ice reservoirs spatial extent, and only at epochs less than 1000 yrs.

Our 2D test suggest that surface chemistry cannot be neglected in the definition of the ice reservoirs and content in disks. However, conclusions are not robust, since surface chemistry networks have in general much larger uncertainties. A more simplified approach based on the spatial extent and abundance of the main precursors of our ices suggest that surface chemistry can be neglected for the size of water ice reservoir, since the contribution is marginal and the
Figure 5.15 – Line flux ratio for $^{13}$CO $J = 2 - 1$ versus C$^{18}$O $J = 2 - 1$, compared with observations. Blue dots are the line observations from Williams & Best (2014), arrows are for upper limits. Green symbols are the results from our series of models, labeled with the different parameter changed with respect to the standard. Models with different $M_{\text{gas}}$ are shown as red squares. The magenta points are the line fluxes of the $J = 3 - 2$ rotational transitions of these isotopologues from the modeling of Miotello et al. (2014) for two extreme $M_{\text{gas}}$ cases, and for the large grain case, that is comparable to our disk models ($f_{\text{large}} = 0.99$). Arrows shows the displacement produced by the isotopologue selective photodissociation.
definition of the ice reservoir will be unaffected. The same conclusion does not hold for other ices such as CO$_2$, where an important contribution (up to a dex in terms of relative abundance), can affect the content of this species in the correspondent ice reservoir. However, the spatial extent of CO$_2$ ice reservoir is not affected by the inclusion of these processes.

The simplified description of ice lines based on the equilibrium relation is quite reliable for the total mass included in the ices, but not for the gas column density beyond 1 au for water and 50 au for CO. Different disk parameters will produce clear signatures on the ALMA line cubes of gas residing above the ice reservoirs, such as CO and isotopologues. Each disk property produces a clear signature on the length of the butterflies of CO isotopologues, and models with high continuum opacity e.g. $d/g = 1$ will have smaller branches with the same length for all three isotopologues, while optically thin models with e.g. $a_{pow} = 2$ will have longer butterfly branches in the C$^{18}$O cube (contrary to the standard model). Models with an extremely high cosmic ray ionization rate, will have longer butterflies and larger difference in the lengths between the three isotopologues.

Line ratios between the CO isotopologue line fluxes suffer from strong degeneracy with several disk parameters. The ratios will line up in a log-log plot. Beside the known effect of selective photodissociation, mass estimates from CO isotopologues line ratios will not be more accurate than a factor 10 unless dust properties are well constrained.
Appendix

A.1 Standard disk plots

Figure 5.16 – Standard disk model plots. Top left density. Top right average dust grain size in μm. Bottom left standard gas temperature. Bottom right standard dust temperature.
Figure 5.17 – Standard disk model abundances plots. Left plots gas phase abundance, right plots ice phase abundance. First row water. Second row CO. Third row CO$_2$. Fourth row NH$_3$. Last row CH$_4$. 

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Fig. 5.17 – continued
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A.2 Surface density computation

We compute the surface density, numerically integrating from the surface downwards to the midplane. The density of each grid point is multiplied by the vertical distance between grid points

$$N_{\text{species}} = \sum_{i=0}^{Nz} n_{\text{species},i} \cdot \Delta z_i$$

In order to include the criteria of Min et al. submitted, we simply assumed that $n_{\text{species}} = 0$ when $P_{\text{species}}/P_{\text{vapor}} > 1$. Similarly we assume that $n_{\text{species}} = 0$ for $T_{\text{gas}} \leq 20$ K and $N_H > 1.3 \cdot 10^{32}$ g/cm$^{-2}$, according to Williams & Best (2014).

A.3 ALMA velocity channels branches length measurement

We measured the length of the butterflies in the ALMA simulations scanning through the data cubes along declination direction (y-axis) and picking the maximum value at each slice, excluding the first 46 pixels along Right Ascension direction (x-axis). For the 30 closest slices to the central pixel (correspondent to the central star), we imposed as “x” coordinate of the maximum the position of the central star. Between these selected points, we perform a quadratic fit using the python package polyfit$^4$ and we measure the length of the final inferior arc because it is the brighter one (disk is inclined of 30°). The length of the arc is based on numerical integration (Eq. 5.9)

$$l_{\text{arc}} = \sum_{i=0}^{n} \sqrt{(\Delta \alpha_{\text{fit},i})^2 + (\Delta \delta_i)^2}$$

The arc length $l_{\text{arc}}$ is the sum of the connectors between the pixels through which the half-parabolic arc passes. Each segment is defined by a displacement along Right Ascension $\Delta \alpha$ (x-axis), computed from the fitting function, and declination $\Delta \delta$ in arcseconds (Fig. 5.18).

$^4$ http://docs.scipy.org/doc/numpy/reference/generated/numpy.polyfit.html
Figure 5.18 – Example of arc length measurement on a lower branch of a butterfly. Blue line connect the selected data points (blue squares), yellow is the parabolic fit. The zoom show how we select the $\Delta \delta$ and $\Delta \alpha$ for the arc measurement.
Chapter 5 – Ice lines and disk structure in protoplanetary disks

A.4 Additional tables

Table 5.4 – Molecular cloud physical conditions adopted in our code

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<th>Parameter</th>
<th>Symbol and unit</th>
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<td>Dust temperature</td>
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<td>Grain size (monosize)</td>
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<tr>
<td>Cosmic ray ionization rate</td>
<td>$\zeta_{\text{CR}}$ [s$^{-1}$]</td>
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All quantities are taken from McElroy et al. (2013)
Table 5.5 – Ice test

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<tr>
<td>OH$^#$</td>
<td>2.587·10$^{-12}$</td>
<td>6.196·10$^{-14}$</td>
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</table>

Tiny differences between the two models are purely numerical. $^#$ symbol is for the ices.
A.5 ALMA simulations

We perform ALMA line observations using the code CASA in configuration 6, adopting the coordinate of DN Tau (\( \alpha : 04h35m27.375s; \delta : +24\degree14'58.93'' \); from SIMBAD), a distance of 140 pc (Pontoppidan et al. 2010a), and assuming an inclination of 30\(^\circ\).

Figure 5.19 – ALMA channel maps for \(^{12}\)CO \( J=3-2 \) for our standard disk model. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.

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6 http://simbad.u-strasbg.fr/simbad/
Figure 5.20 – Same plot as 5.19 but for $^{13}$CO $J=3-2$. 
Figure 5.21 – Same plot as 5.19 but for C^{18}O \( J=3 \rightarrow 2 \).
### A.5 ALMA simulations

Table: ALMA channel maps for $^{12}$CO $J=3-2$ for our disk model with $\alpha_{\text{pow}} = 2.0$. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.

#### Figure 5.22

- ALMA channel maps for $^{12}$CO $J=3-2$ for our disk model with $\alpha_{\text{pow}} = 2.0$. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.
Figure 5.23 – Same plot as 5.22 but for $^{13}\text{CO} \ J=3-2$. 
Figure 5.24 – Same plot as 5.22 but for C$^{18}$O $J=3\rightarrow2$. 

A.5 ALMA simulations
Figure 5.25 – ALMA channel maps for $^{12}\text{CO} \ J=3-2$ for our disk model with dust-to-gas $= 1.0$. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.
Figure 5.26 – Same plot as 5.25 but for $^{13}$CO $J=3-2$. 
Figure 5.27 – Same plot as 5.25 but for C$^{18}$O $J = 3 - 2$. 
Figure 5.28 – ALMA channel maps for $^{12}$CO $J = 3 − 2$ for our disk model with $a_{\text{max}} = 10$ cm. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.
Figure 5.29 – Same plot as 5.28 but for $^{13}$CO $J = 3 - 2$. 
Figure 5.30 – Same plot as 5.28 but for C^{18}O $J=3-2$. 
Figure 5.31 – ALMA channel maps for $^{12}$CO $J = 3 - 2$ for our disk model with $\zeta_{\text{CR}} = 1.7 \cdot 10^{-12}$ s$^{-1}$. Cycle 3, configuration 6, total integration time 48 hrs. Coordinates are the one for DN Tau.
Figure 5.32 – Same plot as 5.31 but for $^{13}$CO $J=3-2$. 
Figure 5.33 – Same plot as 5.31 but for C^{18}O $J=3–2$. 
A.6 CO isotopologues lines emitting regions

Figure 5.34 – Line emitting regions for CO isotopologues $J=2-1$ and $J=3-2$ transitions in the different models. Each contour include the 15-85 % of the radially and vertically integrated line flux. (a) standard model, (b) $d_{\text{pow}} = 2$, (c) $d/g = 1$, (d) $d_{\text{max}} = 10$ cm, (e) $\zeta_{\text{CR}} = 1.7 \cdot 10^{-12}$ s$^{-1}$. Green dashed line is for the bolometric extinction at 1 mag. Purple dot-dashed is for the CO ice line based on abundance criterium.