Snow-lines can be thermally unstable

James E. Owen⋆
Astrophysics Group, Department of Physics, Imperial College London, Prince Consort Rd, London, SW7 2AZ, UK

11 May 2020

ABSTRACT
Volatiles species in protoplanetary discs can undergo a phase change from vapour to solid. These “snow-lines” can play vital roles in planet formation at all scales, from dust coagulation to planetary migration. In the outer regions of protoplanetary discs, the temperature profile is set by the absorption of reprocessed stellar light by the solids. Further, the temperature profile sets the distribution of solids through sublimation and condensation at various snow-lines. Hence the snow-line position depends on the temperature profile and vice-versa. We show that this coupling can be thermally unstable, such that a patch of the disc at a snow-line will produce either run-away sublimation or condensation. This thermal instability arises at moderate optical depths, where heating by absorption of reprocessed stellar light from the disc’s atmosphere is optically thick, yet cooling is optically thin. Since volatiles in the solid phase drift much faster than volatiles in the vapour phase, this thermal instability results in a limit-cycle. The snow-line progressively moves in, condensing volatiles, before receding, as the volatiles sublimate. Using numerical simulations, we study the evolution of the CO snow-line. We find the CO snow-line is thermally unstable under typical disc conditions and evolves inwards from ∼50 to ∼30 AU on timescales from 1,000-10,000 years. The CO snow-line spends between ∼10%−50% of its time at smaller separations, where the exact value is sensitive to the total opacity and turbulent viscosity. The evolving snow-line also creates ring-like structures in the solid distribution interior to the snow-line. Multiple ring-like structures created by moving snow-lines could potentially explain the sub-structures seen in many ALMA images.

Key words: protoplanetary discs — astrochemistry

1 INTRODUCTION
Protoplanetary discs are composed of gas, which typically drives the dynamics, and solids, which can move with respect to the gas. Ultimately, it is the solids that are the building blocks from which planets form. The composition of the solids also varies strongly with position in the disc. As one moves to larger radii, volatile species (e.g. water, carbon dioxide, ammonia and carbon monoxide) are able to condense out of the vapour phase and into the solid phase, significantly enhancing the mass in the solids (e.g. Hayashi 1981; Stevenson & Lunine 1988; Öberg et al. 2011; Booth et al. 2017).

Since the condensation/sublimation of volatile species is a phase change, it happens over narrow ranges of temperature. In the context of protoplanetary discs this leads to rather abrupt changes in the solid density and composition, known as snow-lines (or ice-lines). Snow-lines may play an important role in planet formation. Firstly, one does not just get an increase in solid surface density across the snow-line, but rather a strong local enhancement at the snow-line. This is because the strong concentration gradients allow volatiles in the vapour phase to diffuse back across the snow-line, re-condensing into the solid phase, increasing the solid density locally at the snow-line (e.g. Stevenson & Lunine 1988; Cuzzi & Zahnle 2004; Kretke & Lin 2007). Secondly, the accretion of volatiles in either the vapour or solid phase will result in the sequestration of those elements, either in the planetary core or atmosphere. Therefore, understanding how volatiles are accreted by forming planets will allow us to interpret observations of the composition of exoplanet atmospheres (e.g. Öberg et al. 2011; Madhusudhan et al. 2014; Booth et al. 2017; Tinetti et al. 2018; Booth & Ilee 2019).

The most commonly studied snow-line is the water snow-line. This is because water is one of the most abundant volatiles, resulting in a large solid density change (e.g. Hayashi 1981; Stevenson & Lunine 1988), and it is typically co-located between the terrestrial and giant-planets in our solar-system (e.g. Martin & Livio 2012; Martin & Lubow 2013). However, there are a multitude of other snow-lines, including but not limited to ammonia, nitrogen, carbon diox-

⋆ E-mail: james.owen@imperial.ac.uk
© 2015 The Authors

arXiv:2005.03665v1 [astro-ph.EP] 7 May 2020
The carbon monoxide (CO) snow-line is important in the astronomical context for several reasons. Firstly, CO is also an abundant volatile, resulting in large solid density changes at its snow-line (e.g. Öberg et al. 2011; Madhusudhan et al. 2014). Secondly, CO is commonly used as a tracer of gas in protoplanetary discs through sub-mm observations. Thus, understanding CO’s distribution is crucial to interpreting sub-mm fluxes and images of protoplanetary discs (e.g. Williams & Best 2014). Finally, since the CO snow-line occurs in the outer regions of protoplanetary discs it (or its imprint) has been observed directly (e.g. Qi et al. 2013, 2019).

2 BASIC CONCEPT

Understanding the location, evolution and chemistry of all snow-lines is going to be crucial to our understanding the chemistry of protoplanetary discs, planet formation and ultimately will allow us to interpret the compositions of exoplanet atmospheres. However, current work typically calculates the properties of snow-lines assuming the underlying disc temperature profile is fixed (e.g. Öberg et al. 2011; Booth et al. 2017), or based on simple models that account for viscous heating (e.g. Kretke & Lin 2007; Martin & Livio 2012, 2014). This approximation breaks down in protoplanetary discs, particularly in the outer regions. This is because it is the solid particles that absorb the stellar light and control the temperature of the disc. Therefore, changes in the distribution of solids will change the temperature profile which will change the distribution of solids. This is particularly important at snow-lines as small temperature changes can lead to large changes in the distribution of solids.

In this work we show snow-lines, that occur at moderate optical depths in passively heated discs, are subject to thermal instabilities. Specifically, the snow-lines do not occur at fixed (or secularly evolving) locations as previously thought, but move over large distances in otherwise stationary discs. This thermal instability fits within the picture of previously identified thermal instabilities in classical, active accretion discs, that are more commonly studied in high-energy astrophysics (e.g. Pringle 1981; Faulkner et al. 1983; Lasota 2001) or the earliest phases of star-formation (e.g. Armitage et al. 2001; Zhu et al. 2010; Martin & Lubow 2011, 2013). The fact that many snow-lines are constantly evolving has important consequences for the chemistry of protoplanetary discs, the formation of planetesimals and planets and the interpretation of astronomical observations.

2.1 Qualitative description

A thermal instability requires that the heating-rate is a stronger increasing function of temperature than the cooling rate. If this is the case, a system in thermodynamic equilibrium will be unstable to small temperature perturbations. For example, if the temperature increases slightly, then as the heating rate is a stronger increasing function of temperature, the small temperature increase results in a net heating rate, further increasing the temperature. Such an argument equally applies to a small temperature decrease, which leads to net cooling and continued reduction of the temperature.

In the outer regions of a protoplanetary disc, the heating and cooling is almost exclusively set by radiative balance (i.e. viscous heating is negligible). Now consider a region of the disc with a temperature just below that required to sublimate a volatile. A small temperature increase will result in the volatile beginning to sublimate into the gas phase, decreasing the solid abundance. Since it is the solids that dominates the opacity of the disc, and hence the absorption and emission of radiation, the heating and cooling of the disc can be strongly affected by the decrease in solid abundance.

In the outer regions of protoplanetary discs cooling is typically optically thin, hence this decrease in solid abundance will decrease the cooling rate. The heating of the disc arises from absorption of stellar irradiation re-radiated towards the disc mid-plane from the surface layers. Should the absorption of this re-radiated emission also be optically thin then the heating rate will also decrease in an equal fashion to the cooling rate and the disc will be thermally stable. However, should the absorption of this re-radiated emission be at least marginally optically thick (or not very optically thin), then even though the solid abundance has decreased the disc will still absorb most of this re-radiated stellar light, hence the heating rate will remain unchanged. In this case, a small increase in disc temperature will result in drop in the cooling rate and a practically unchanged heating rate, leading to a net heating rate. Thus, the disc will increase in temperature leading to runaway sublimation of all the volatiles in the solid phase.

The above argument also indicates a crucial requirement for this thermal instability: that the absorption of re-radiated stellar light and emission by the disc’s mid-plane must occur at different optical depths. Namely, the absorption should be more optically thick than the cooling. Such a situation is natural in the outer regions of protoplanetary discs. Stellar irradiation of the surface layers of discs results in a “super-heated” surface-layer that is typically a factor of 4 hotter than the mid-plane (e.g. Chiang & Goldreich 1997). Since solid opacity increases with the increasing temperature of the radiation field, the optical depth to the re-radiated stellar light is naturally larger than that of the emission from the disc’s mid-plane. Hence, an important aspect of this instability when it comes to modelling is that it requires a...
non-grey treatment of not just the stellar radiation, but also the re-radiated stellar light from the disc’s surface layers and the disc’s mid-plane. If the disc is too optically thin, then the heating and cooling rate both respond linearly to the change in solid abundance and there is no instability. Further, if the disc is too optically thick the heating and cooling rates are essentially independent of the solid abundance\(^1\). Since the water snow-line occurs in regions of the disc that are optically thick under standard conditions (and where viscous heating is important – Kretke & Lin 2007 and Martin & Lubow 2011), it is likely to be thermally stable. However, we speculate that snow-lines in the outer regions (e.g. CO, CO\(_2\), NH\(_3\)) are thermally unstable.

2.2 Quantitative description

In this sub-section we remain agnostic to the specific volatile species and discuss the requirements in general terms. A thermal instability in a disc requires:

\[
\frac{\partial \log Q_+}{\partial \Sigma_m} > \frac{\partial \log Q_-}{\partial \Sigma_m} \tag{1}
\]

where \(Q_+\) and \(Q_-\) are the heating and cooling rates of the disc per unit area respectively and \(\Sigma_m\) is the mid-plane temperature. Taking the interior of the disc to be isothermal, with a temperature \(T_m\), and containing a surface density of solids \(\Sigma_d\), the cooling rate is (c.f. Dulmond et al. 2001):

\[
Q_- = 2 \sigma T_m^4 \int \frac{\kappa_v(T_m) [1 - \exp(-\Sigma_d \kappa_v/2)]}{\int \kappa_v B_v(T_m) \text{d}v} = 2 f_{\text{em}} \sigma T_m^4 \tag{2}
\]

where \(B_v\) is the Planck function as a function of frequency (\(v\)), \(\kappa_v\) is the solid opacity as a function of frequency, \(\Sigma_d\) is the dust surface density and \(f_{\text{em}}\) represents the cooling rate scaled to that of a pure black-body. The factor of 2 comes from the two sides of the disc. Further the heating rate is:

\[
Q_+ = f_{\text{surf}} \int \frac{\kappa_v B_v(T_{\text{surf}}) [1 - \exp(-\Sigma_d \kappa_v/2)]}{\int \kappa_v B_v(T_{\text{surf}}) \text{d}v} = f_{\text{abs}} f_{\text{surf}} \tag{3}
\]

where \(f_{\text{surf}}\) is the fraction of the stellar light re-radiated towards the mid-plane by the surface layers, \(T_{\text{surf}}\) is the temperature of the super-heated surface layers and \(f_{\text{abs}}\) represents the fraction of the re-radiated emission from the surface layers that is absorbed by the mid-plane.

Now, in the optically thick limits \(\Sigma_d \kappa \gg 1\), \(f_{\text{em}}\) and \(f_{\text{abs}}\) are unity and there is no thermal instability (unless \(\partial \log F_{\text{surf}}/\partial \log T_m > 4\) which appears unlikely as the solid abundance decreases with increasing temperature at the snow-line), as expected from our qualitative discussion above.

In the fully optically thin limit, e.g. \(\Sigma_d \kappa \ll 1\) at all relevant frequencies, \(f_{\text{em}} \rightarrow \Sigma_d \kappa_p(T_m)/2\) and \(f_{\text{abs}} \rightarrow \Sigma_d \kappa_p(T_i)/2\) (e.g. Chiang & Goldreich 1997), where \(\kappa_p\) is the Planck mean opacity. As expected, both the heating and cooling rate linearly depend on \(\Sigma_d\) in the optically thin limit. Thus, the only way to obtain a thermal instability requires the opacity changes due to the composition changes of the solid particles. While not implausible, the magnitude of the changes required \(\partial \log \kappa_p(T_m)/\partial \log T_m \lesssim -4\), means such a scenario may require a particularly special snow-line.

However, at intermediate optical depths satisfying Equation 1 becomes possible. To demonstrate this explicitly, while keeping our discussion agnostic about the species, we assume absorption and emission due to the solids can be described by geometric optics. Such that the opacity of a spherical grain, of size \(s\), internal density (\(\rho_i\)), as a function of wavelength (\(\lambda\)) is given by:

\[
\kappa_\lambda(s) = \frac{3 Q(s, \lambda)}{4 \pi s} \tag{4}
\]

where \(Q(s, \lambda)\) is the absorption efficiency. In the geometric limits \(Q = 1\) when \(\lambda < 2 \pi s\), and \(Q = (s/2 \pi \lambda)^{\beta}\) when \(\lambda > 2 \pi s\), where \(\beta\) is the Rayleigh index.

Now consider a scenario where the solid abundance drops from \(\Sigma_d\) to \(1/4 \Sigma_d\) across the snow line at a temperature of \(T_{\text{snow}}\), with a width of 5% of the snow-line temperature\(^2\). Calculations for physical parameters are shown in Section 3. The surface temperature \(T_{\text{surf}} = 4T_{\text{snow}}\). Figure 1 shows the heating and cooling rates as a function of temperature at a very high, moderate and very low optical depth. We choose a particle size that satisfies \(2 \pi s = b/T_{\text{ce}}\) where \(b\) is Wein’s constant, use an internal density 1.25 g cm\(^{-3}\) and adopt \(\beta = 1\). This Figure shows (as discussed above) there is only one point at which heating balances cooling for the very high and very low optical depths all of which are thermally stable \((\partial \log Q_+ / \partial T_m < \partial \log Q_- / \partial T_m)\). However, the moderate optical depth case shows three points at which heating balances cooling with the solution at a temperature of \(T_{\text{snow}}\) being thermally unstable \((\partial \log Q_+ / \partial T_m > \partial \log Q_- / \partial T_m)\).

We note that provided the optical depths to cooling are moderate, the presence of a thermal instability is rather insensitive to the change in solid density, and how quickly this change happens, provided the transition occurs over a range of temperatures \(\Delta T \ll T_{\text{snow}}\).

2.3 Existence of a Limit Cycle

One question we must now explore is how this thermal instability manifests in real protoplanetary discs. In the vicinity of the snow-line at moderate optical depths there are two possible temperature solutions at higher or lower temperatures than \(T_{\text{snow}}\), and further there must be a radius in the disc where its temperature “jumps” from the hot solution to the cold solution. However, a discontinuity in the temperature of the disc is not physical. Thus, by analogy with previously identified thermal instabilities in accretion discs it is likely to manifest itself as a limit-cycle, where the snow-line evolves in the disc. Therefore, a given radius in the disc will spend some of its time on the hot solution and some of its time on the cold solution.

A limit-cycle occurs when there exists a forbidden range of accretion rates (e.g. Pringle 1981). In the context of our snow-line, we consider this to be a mass-flux of the volatile. This can either occur in the solid phase via radial drift, or in the gas-phase via advection along with the accreting gas.
If the solids have grown sufficiently, such that radial drift is faster than gas advection, then a range of forbidden mass-fluxes of volatiles can exist. We will have a high volatile mass-flux when the disc is at the cold temperature solution as the volatiles are in the solid phase, and a low-mass flux when the disc exists at the hot temperature solution. If we feed the disc at a volatile mass flux that exists between the two allowed mass-fluxes then no steady-state can exist, and the disc will evolve through a limit-cycle. With the disc spending sometime in the cold, high accretion rate phase, and another fraction of the time in the hot, low accretion rate phase.

2.3.1 Construction of an “S-curve”

Consider a surface density of a given volatile \( \Sigma_v \) if the volatile is in the solid phase the mass-flux is approximately (e.g. Takeuchi & Lin 2002):

\[
M_v^{\text{ice}} = 2 \pi R \Sigma_v \tau_s \left( \frac{\log P}{\log R} \right)^2 \frac{H}{R} \nu_K
\]

(5)

where \( \tau_s \) is the Stokes number (or dimensionless stopping time) of the solid particles, \( H \) is the disc scale height and \( P \) the mid-plane pressure. Whereas if the volatile is in the solid phase the mass-flux is approximately:

\[
M_v^{\text{vapour}} = 3 \pi R \Sigma_v \alpha \left( \frac{H}{R} \right)^2 \nu_K
\]

(6)

Therefore, comparing Equations 5 & 6, and noting the logarithmic pressure derivative is of order unity, we see the mass-flux in the ice-phase will be significantly higher than that in the vapour phase if the solids are undergoing radial drift (i.e. \( \tau_s \gg \alpha \)). Since this is the standard case for the outer regions of protoplanetary discs (e.g. Birnstiel et al. 2012), we expect this to be the norm.
Volatile Mass-flux [arb. units]

Temperature (T) [T\text{snow}]

Figure 3. A sketch of a simple model for the limit-cycle. The top plot shows the S-curve of volatile surface density against volatile mass-flux. The bottom plot shows the disc temperature as a function of volatile surface density. The volatile surface density is scaled to a value to give a Planck optical depth of unity to radiation with a temperature of T_{\text{snow}}. The solid blue lines represent thermally stable solutions, the dotted red lines represent thermally unstable solutions. No thermally stable states exist in the “forbidden region” of volatile mass-flux. The purple arrows sketch out the limit-cycle the disc’s region will follow in both mass-flux and temperature. This schematic plot shows the limit cycle exists at moderate optical depths.

3 MODEL - THE CO SNOW-LINE

In Section 2 we deliberately kept the discussion arbitrary, to demonstrate the robustness of the thermal instability. However, in order to run simulations that are applicable to real protoplanetary discs, we must be specific. The CO snow-line is observed to occur in the outer regions of protoplanetary discs (Qi et al. 2013; Guidi et al. 2016; Qi et al. 2019), thus we initially choose to explore the CO snow-line in this work.

3.1 Disc temperature calculation

Our mechanism requires that we dynamically evolve the temperature structure of the disc, along with the surface densities and ice/vapour compositions. Further, our discussion in Section 2 requires this calculation takes into account the non-grey nature of the radiative transfer. The typically used hybrid-grey FLD method (e.g. Kuiper et al. 2010; Bitsch et al. 2013) or other common 1+1D methods (e.g. D’Alessio et al. 1998, 2001), do not capture the physics of this thermal instability. The coupling of the thermal evolution of the disc to its dynamical evolution requires a simplified radiative transfer scheme. Therefore, we adopt the two-layer model (e.g. Chiang & Goldreich 1997; Chiang et al. 2001; Dullemond et al. 2001), where the disc is separated into a “super-heated” atmosphere (heated by direct irradiation from the star) at a temperature of T_{\text{atm}} and an interior (heated by the reprocessed stellar irradiation emitted by the disc’s atmosphere) at a temperature of T_{\text{int}}. Within the interior and atmosphere the temperatures are taken to be constant and independent of height. The interior is taken to be in vertical hydrostatic equilibrium with this temperature profile. The transition from the interior to the atmosphere occurs at the photosphere to stellar irradiation (h).\footnote{Note in this work we use the opposite, but more common, convention to Chiang et al. (2001), where we use H for the disc’s scale height and h for the height of the photosphere.} This scheme has been shown to accurately capture the nature of the radiative transfer problem when compared to more complete radiative transfer solutions (e.g. Dullemond & Natta 2003; Rafikov & De Colle 2006).

The two-layer scheme as proposed by Chiang & Goldreich (1997), was later modified by Chiang et al. (2001) and Dullemond et al. (2001). We build on these previous works and present a slightly different formalisation, suitable for coupling within a dynamical calculation. To avoid slow integration over frequency (e.g. Equations 3 & 2) we follow (Chiang et al. 2001) and consider three average radiation fields and mean opacities. Firstly, the opacity of the atmosphere to stellar light is described by a Planck-mean opacity at the stellar temperature ($\kappa_p(T_\ast)$). Secondly, the opacity...
to radiation at the disc’s atmosphere’s temperature is described by a Planck-mean opacity at the temperature of the atmosphere ($\kappa_p(T_{\text{atm}})$). Finally, we approximate the opacity to radiation at the interior’s temperature by a Planck-mean opacity at $T_m$.

These simplifications allow the temperature of the atmosphere to be written as:

$$T_{\text{atm}} = T_r \left( \frac{R_s}{R} \right)^{1/2} \left( \frac{\phi \kappa_p(T_r)}{4 \kappa_p(T_{\text{atm}})} \right)^{1/4}$$

(7)

where $R_s$ is the stellar radius, $R$ is the cylindrical radius from the star and $\phi$ is the fraction of the stellar disc seen by the atmosphere which we set to 1/2. The heating rate per unit area (including both sides of the disc) is given by:

$$Q_+ = \phi \left[ 1 - \exp \left( - \frac{\Sigma \kappa_p(T_{\text{atm}})}{2} \right) \right] \left( \frac{R_s}{R} \right)^2 \sigma T_r^4 \sin \alpha$$

(8)

where $\alpha_f$ is the “flaring” angle - i.e. the grazing angle between incoming stellar irradiation and the photosphere. The factor of a half in the exponential comes from the fact the irradiation from the disc’s surface only traverses half of the disc’s surface density before it reaches the mid-plane.

Finally, the cooling-rate per unit area (including both sides of the disc) is:

$$Q_- = 2 \left[ 1 - \exp \left( - \frac{\Sigma \kappa_p(T_{\text{atm}})}{2} \right) \right] \sigma T_m^4$$

(9)

3.1.1 Calculation of the flaring angle

Calculation of the flaring angle is non-trivial. An implicit ray-tracing can result in numerical instabilities (e.g. Dullemond 2000). In the limit that $\alpha_f$ is small, the definition of the flaring angle (e.g. Chiang & Goldreich 1997) becomes:

$$\alpha_f = \left( \frac{3}{4\pi} R_s + R \frac{d}{dR} \left( \frac{h}{R} \right) \right)$$

(10)

Locally, ignoring shadowing (see Section 5.2 for a discussion of shadowing), the flaring angle is also defined by, (Dullemond et al. 2001):

$$\frac{\kappa_p(T_s)}{\alpha_f} \int_h^\infty \rho(z)dz = 1$$

(11)

Assuming the vertical density structure is Gaussian (as true for an isothermal disc in hydrostatic equilibrium) this can be solved to give, (Dullemond et al. 2001):

$$1 - \text{erf} \left( \frac{h}{\sqrt{2}H} \right) = \frac{2\alpha_f}{\Sigma_d \kappa_p(T_s)}$$

(12)

We note in passing that Equations 10 & 12 can be combined to create an ODE for $h$. However, in practice solving this ODE requires knowing the height of the photosphere at the inner boundary. We find that we cannot accurately estimate this boundary condition such that integration of the ODE provides a numerically stable solution for $\alpha_f$. Therefore, following Dullemond et al. (2001) we note that $h$ is a smoothly varying function and write that $\partial h/\partial R \approx \gamma - 1$ in Equation 10, where $\gamma$ is the “flaring index of the disc” formally defined by:

$$\gamma = \frac{d \log h}{d \log a}$$

(13)

Following both Chiang et al. (2001) and Dullemond et al. (2001), we note that $h/H$ is an extremely slowly varying function (roughly varying from 5 to 3 from $< 0.1$ AU to $> 100$ AU); thus, we approximate $\gamma$ as:

$$\gamma \approx \frac{d \log H}{d \log a}$$

(14)

so the flaring angle becomes:

$$\alpha_f \approx \left( \frac{3}{4\pi} R_s + (\gamma - 1) \frac{h}{R} \right)$$

(15)

where the combination of Equation 12 & 15 can be solved to find the value of $h$ and hence $\alpha_f$. We do this using Brent’s root finding method with a relative tolerance of $10^{-6}$. This approximate form of the flaring index allows us to include both changes from the temperature profile and surface density. In the case that the flaring index does not change, this give us that the heating rate is $\propto T_{\text{atm}}^{1/2}$ used previously.

3.1.2 Latent Heat

Any phase change carries with it an exchange of internal energy and thermal energy. The sublimation of ice requires the absorption of thermal energy, cooling the surroundings. Thus the act of sublimation is thermally stabilising. Therefore the act of sublimation is thermally stabilising. The absorption/release of latent heat has the potential to stabilise our thermal instability. However, due to the short thermal timescales in the outer regions of protoplanetary discs this turns out not to be the case (at least for the CO snow-line). This result can be seen from the following analysis.

The heating rate per unit area due to latent heat can be written as:

$$Q_{\text{lat}} = L_{\text{sub}} \left( \frac{M_{\text{CO}}}{2\pi R^2} \right) \frac{dX_{\text{ice}}}{dR}$$

(16)

where $L_{\text{sub}}$ is the latent heat of sublimation, $M_{\text{CO}}$ is the CO mass-flux and $X_{\text{ice}}$ is the fraction of the volatile species in the ice phase. The radial derivative of the ice-mass fraction can be written as:

$$\frac{dX_{\text{ice}}}{dR} = \frac{dX_{\text{ice}}}{dT_m} \frac{dT_m}{dR}$$

(17)

where the derivative of the ice-mass fraction as a function of temperature is set by the dynamics of the phase change (see Section 3.2). Measurements of the latent heat of CO for sublimation temperatures closer to 50-60 K indicate a value of $\sim 3 \times 10^9$ erg g$^{-1}$ (Stephenson & Malanowski 1987). While the sublimation temperature under protoplanetary conditions is closer to 20-30 K, one would not expect the value of the latent heat to be dramatically different.

We can estimate the role of cooling due to sublimation by considering its ratio with respect to radiative cooling (in the limit $\tau < 1$):

$$\frac{Q_{\text{lat}}}{Q_{\text{cool}}} = \frac{L_{\text{sub}} X_{\text{ice}} M_{\text{CO}}}{2 \pi R^2 \tau \sigma T_m^4} \frac{d \log X_{\text{ice}}}{d \log T_m}$$

$$\approx \left( \frac{R}{50 \text{ AU}} \right)^{-2} \left( \frac{T_m}{25 \text{ K}} \right)^{-4}$$

(18)

(19)

Our CO sublimation model indicates an appropriate value
of $\partial \log X_{\text{co}} \partial \log T_{\text{in}} \sim 10-30$ in the region of the snow-line. Therefore, even with our quite large choice of the CO mass flux (and the fact that the snow-line is only thermally unstable at intermediate optical depths) we find that latent heat is unimportant at the $\sim 10^{-3}$ level, and will not stabilise our thermal instability. This is born out when we explicitly include latent heat in the calculation of our CO S-curve and find it’s unimportant. In our numerical simulations in Section 4 we do not include latent heat for simplicity.

### 3.1.3 Opacities

The precise details of CO opacities has not been explored in as much detail as other ices (e.g. Water) or silicates. Therefore, we proceed to continue to work with opacities motivated from geometric optics. Firstly, for simplicity we consider an opacity law than encodes the minimum physics, namely we ignore the particle size dependence on the opacity and assume the Planck-mean opacity is given by:

$$\kappa_p = 10 \text{ cm}^2 \text{ g}^{-1} \left( \frac{T}{10 K} \right)$$  \hspace{1cm} (20)

We note that this is opacity per unit mass of solids, not per unit mass of gas (+ dust). Therefore, for a dust-to-gas mass ratio of 0.01 this opacity corresponds to the “standard” sub-mm opacity of 0.1 cm$^2$ g$^{-1}$.

We can explore the exact dependence on temperature and particle size by taking more considerations from geometric optics. Further, assuming an MRN grain-size distribution with the number density distribution scaling as $n(s) \propto s^{-3.5} ds$, up to a maximum size of $s_{\text{max}}$, the opacity is dominated by the smallest grains which we set to 0.1 $\mu$m. However, the mass is dominated by the largest grains. Such choices motivate a phenomenological opacity functional form of:

$$\kappa_p(s_{\text{max}}, T) = \kappa_0 \left( \frac{s_{\text{max}}}{1 \text{ cm}} \right)^{-1} \left( \frac{T}{10 K} \right)^{\beta - 3.5}$$  \hspace{1cm} (21)

with $\beta = \pi s_{\text{max}} T / h$, roughly the ratio of the mean photon wavelength to the size of the particle ($h$ again is the constant in Wein’s displacement law). This form correctly reproduces the limits of the parameter space and the form of the opacity function. For $\beta = 1 \& 2$, we find $\kappa_0 = 0.9 \text{ cm}^2 \text{ g}^{-1}$ & 0.7 cm$^2$ g$^{-1}$ produces a good match to numerically calculated mean opacities respectively. The choice of this functional form over tabulated opacities is purely one of numerical efficiency. Finally, for the choice of opacity in the atmosphere of the disc ($\kappa_p(T_{\text{in}})$) we assume only small particles are present (due to vertical settling) and set $s_{\text{max}} = 1 \mu$m in the disc’s atmosphere.

### 3.2 CO ice-vapour chemistry

Our CO sublimation model follows Booth et al. (2017) and Booth & Ilee (2019), which itself is based on the models of Hollenbach et al. (2009). Booth et al. (2017) explicitly demonstrated the timescale for small solid particles (e.g. less than a few centimetres) to reach an adsorption-desorption equilibrium is short compared to the relevant transport timescale in a protoplanetary disc. This conclusion is in agreement with the results of Piso et al. (2015) who showed only particles larger $\sim 0.5$ cm drifting appreciably while sublimating. Therefore, we solve for the equilibrium CO ice abundance by balancing the thermal adsorption and desorption rates in the mid-plane of the disc. The thermal desorption rate per grain is given by:

$$\Gamma_d = 4 \pi \omega N_d f_i$$  \hspace{1cm} (22)

where $N_d = 1.5 \times 10^{15}$ cm$^{-2}$ is the number of binding sites per unit area, $f_i$ is the fraction of binding sites covered by CO ice, $s_0$ is the size of the grain and $R_d$ is the desorption rate per molecule given by:

$$R_d = v_i \exp \left( \frac{T_{\text{bind}}}{T_{\text{in}}} \right)$$  \hspace{1cm} (23)

with $v_i$ the vibrational frequency of the CO molecule in the potential well of the dust’s surface given by, (Hollenbach et al. 2009):

$$v_i = 1.6 \times 10^{11} \text{ s}^{-1} \frac{T_{\text{bind}}}{m_{\text{CO}}/\hbar}$$  \hspace{1cm} (24)

where $T_{\text{bind}}$ is the binding temperature of the molecule to the surface in Kelvin. We use a value of $T_{\text{bind}} = 960$ K (Aikawa et al. 1996), which sets the sublimation temperature to $\sim 25$ K under typical disc conditions.

Adsorption arises due to grain-molecule collisions; if all these collisions result in adsorption of the molecule, then the adsorption rate per grain is:

$$\Gamma_a = n_{\text{CO},\nu} \pi s_0^2 v_i$$  \hspace{1cm} (25)

where $n_{\text{CO},\nu}$ is the number density of CO molecules in the vapour phase and $v_i$ is their thermal velocity. For the grain size we use $s_0 = 0.1 \mu$m; while in our work we do include a prescription for grain size we follow Booth et al. (2017), who argue using the work of Stammmer et al. (2017) that for a size distribution of $n(s) \propto s^{-3.5} ds$ the adsorption-desorption equilibrium was set by the small grains (which dominate the total grain surface area), while the mass is dominated by the large grains. To find the CO ice and vapour fractions we simply equate the adsorption rate to the desorption rate.

### 3.3 Limit Cycle

Armed with the above methods for calculation of the disc’s temperature and CO vapour and ice fractions we can calculate the real limit-cycle for the CO snow-line provided $\gamma$ is known. Here we simply pick a value for the temperature gradient ($d \log T_{\text{in}}/d \log R = -0.45 \& -0.55$) and calculate the S-curve for the CO snow-line at 50 AU. We assume a solar-mass pre-main-sequence star with $T_\ast = 4000$ K and $R_\ast = 1.43 R_\odot$. For the ice-phase the particles are taken to have a stokes number of 0.05 (roughly 0.3 mm in size for a typical disc) and we assume a viscous $\alpha = 10^{-3}$. The gas surface density profile is also taken to be $S \propto R^{-3}$, and the dust (excluding CO ice) surface density is taken to be 0.01 g cm$^{-2}$. The above choices do not affect the existence of the limit-cycle and the thermal instability, but do affect the quantitative properties. Figure 4 shows the CO S-curve. We have checked that the latent heat from CO sublimation does...
not change the S-curve at a bigger that the $10^{-5} - 10^{-6}$ level. Figure 4 bears a similarity to our simple example in Section 2 where there is a hot, vapour dominated, low mass-flux branch and a cold, ice dominated, high mass-flux branch. Unlike “classical” thermal instabilities, the size of the forbidden range of mass-flux is not set by the physics of the instability, rather the ability of the dust to drift relative to the gas. In a standard viscous accretion disc this is simply parametrised by the ratio of the Stokes number to the viscous alpha.

However, the existence of a limit cycle and thermal instability is not fixed to the assumption of a viscous accretion disc. Rather it arises due to the non-grey radiative-transfer of how a protoplanetary disc is heated and the ability of the solids to drift relative to the gas. Therefore, in the case that protoplanetary accretion is wind-driven (e.g. Bai & Stone 2013; Gressel et al. 2015; Bai et al. 2016), provided the dust has grown to a sufficient size to drift relative to the gas, an S-curve and limit cycle will also exist.

4 NUMERICAL CALCULATIONS

Our discussion so far has focused on showing equilibrium steady-state solutions are unstable, and on the calculation of S-curves at fixed radii. Drawing on the analogy with previous thermal instabilities, we expect the disc to evolve through an ice-dominated “high-mass-flux” state and a vapour-dominated “low-mass-flux” state, where the snow-line propagates through the disc. To calculate the disc’s evolution and response to the thermal instability we perform numerical calculations where we couple the thermal calculation of the disc to the evolution of the solids and the ice-vapour partitioning of CO. To isolate different effects we fix the surface densities of gas, dust and CO as well as the maximum particle size at the outer boundary. This means, if there was no thermal instability, the simulation would then be expected to reach a steady state. We also work within the framework that the protoplanetary disc is a viscous accretion disc.

4.1 Methods

The numerical calculation for the evolution of the surface-densities follows the first-order in time, second-order in space algorithm presented in Owen (2014). This is used to update the surface densities of CO-free dust, CO-ice and CO vapour through the standard thin-disc advection-diffusion equation for the surface density of species $\Sigma_i$:

$$\frac{\partial \Sigma_i}{\partial t} = \frac{1}{R} \frac{\partial}{\partial R} \left[ R \Sigma_i v_i - \nu R \Sigma_i \frac{\partial}{\partial R} \left( \frac{\Sigma_i}{\Sigma} \right) \right]$$

(26)

where $v_i$ is the velocity of the species, and $\nu$ is the kinematic viscosity\(^5\). The velocity is set to the gas velocity for the CO-vapour. The dust-velocity for both the CO-free dust and CO-ice is (from the standard terminal velocity approximation in thin discs Takeuchi & Lin e.g. 2002):

$$v_i = \frac{v_{s,i}}{\tau_s + \tau_{s,i}^{-1}} - \frac{\nu \Omega R}{\tau_s}$$

(27)

with $\tau_s = \pi \rho_{d,max}/2 \Sigma_s$ the Stokes number in the Epstien drag limit, and $\eta$ is a measure of the mid-plane gas pressure gradient given by:

$$\eta = -\frac{d \log P}{d \log R} \left( \frac{H}{R} \right)^2$$

(28)

4.1.1 Gas Evolution

In our scenario where the dust and ice mass fraction is sufficiently small that the dynamical feedback on the gas is negligible, it is unclear whether the gas should evolve in the scenario where its surface density is fixed at the outer boundary. This depends on how you truly interpret the viscous alpha formalism. In the case $v = \alpha_c \Omega R$, if $\alpha_c$ is a fundamental constant then the kinematic viscosity varies as the

---

\(^5\) Hence we are implicitly setting the Schmidt number to unity.
temperature changes and hence the gas-surface density will evolve. However, there is no reason to believe that \( \alpha \) is \textit{truly} constant. Therefore, we choose not to evolve the gas surface density and simply set \( v = v_0 R \), as one would expect from a constant value of \( \alpha \), if the temperature profile followed \( T_m \propto R^{-1/2} \). For, ease of comparison \( v_0 \), is chosen such that if the disc had a temperature of 100 K at 1 AU and it obeys the \( \alpha \) prescription, where \( \alpha \) is the value we quote.

Therefore, in all our calculations the gas-surface density does not evolve and is fixed to follow:

\[
\Sigma_g = \Sigma_0 \left( \frac{R}{R_0} \right)^{-1}
\]  

(29)

4.2 Particle-size evolution

It is well known that mutual collisions between dust particles results in growth in the outer regions of protoplanetary discs (e.g. Brauer et al. 2008; Birnstiel et al. 2010). It is tempting to implement the well-used Birnstiel et al. (2012) dust-size evolution model. This model assumes that the sizes are set by a drift-growth equilibrium in the outer regions of a protoplanetary disc. However, this equilibrium is reached over length scales of \( \sim R \), not length scales where the solid surface density can abruptly change at snow-lines. Implementation of this equilibrium model at the snow-lines results in rather abrupt particle size changes, which are unphysical. Therefore, the temperature evolution is typically solved implicitly and we do the ice-vapour balance inside this implicit solution. This is done so the optical depth is correctly updated. Without this coupling inside the implicit temperature solution. This is done so the optical depth is correctly updated. Without this coupling inside the implicit temperature solution we find numerical instabilities and the radial component of the flux is explicitly included in numerical calculations (Faulkner et al. 1983; Cannizzo 1993). This radial flux is negligible everywhere but at the snow-line. Thus, evolution of the mid-plane temperature follows, (c.f. Owen & Armitage 2014):

\[
C_p \Sigma_m \frac{dT_m}{dt} = Q_{\text{heat}} - Q_{\text{cool}} - 2 \left( \frac{H}{R} \frac{\partial}{\partial R} (F_R) + Q_{\text{background}} \right)
\]

(31)

where \( F_R \) is the radial (cylindrical) radiative flux and \( Q_{\text{background}} \) is a background heating term from the surrounding star cluster. This background heating is set to a value of:

\[
Q_{\text{background}} = 2 \left[ 1 - \exp \left( \frac{\Sigma_d \kappa_R (10 \text{ K})}{2} \right) \right] \sigma_0 T_{10 \text{K}}^{-4}
\]

(32)

In the absence of other heat sources this heating term bathes the disc in a background radiation field of 10 K preventing the disc from becoming too cold in the outer regions.

As the instability we are interested in explicitly occurs at moderate optical depths, applying the radiative diffusion limit for \( F_R \) is not correct. Limited with poor options about how to solve for \( F_R \), we choose flux-limited diffusion. In flux-limited diffusion the flux is written as:

\[
F_R = -\frac{\alpha c \partial E}{\kappa R \partial R}
\]

(33)

where \( E_R = a T_m^4 \) is the radiative energy density, \( c \) is the speed of light, \( \rho_m \) is the mid-plane density and \( \lambda \) is the flux-limiter. The flux-limiter naturally blends the optically thick and thin region with a phenomenological smoothing function. Following Kuiper et al. (2010), we choose:

\[
\lambda = \frac{2 + r}{6 + 3r + r^2}
\]

(34)

with \( r = |\nabla E_R|/(\kappa \rho_m E_R) \), a measure of how optically thick the region is. We are now faced with a choice as to how to interpret \( r \) within our thin disc model as it depends on \( |\nabla E_R| \) rather than \( \partial E_R/\partial R \). Ignoring this fact delivers the wrong approach to the limits. Through experimentation we find that the radial-flux is always sub-dominant (although not negligible) at snow-lines, therefore we crudely approximate \( |\nabla E_R| \) as resulting from its gradient in the vertical direction only; so \( \sim E_R/H \). This allows us to write \( r \approx 4/(\kappa |T_m| \Sigma) \).

None of the above choices are thoroughly satisfactory; however, without a full 2D non-grey solution to the radiative transfer problem this is perhaps the most sensible method. The equations for heating and cooling rates are taken from Equations 8 and 9 respectively. The heating rate depends on \( \gamma \) which in turn depends on the temperature gradient (Equation 14) and the radiative flux term also includes terms that depend on the temperature gradient. Thus, Equation 31 cannot be solved at each annulus independently. Previous works that have employed this method use the \( \gamma \) value from the previous radial grid point, and update it only every two radial grid points (Chiang et al. 2001). We find this approach leads to large errors at opacity jumps (e.g. at snow-lines) and non-continuous temperature structures. Therefore, we evaluate \( \gamma \) using 4th order central numerical differencing of Equation 14, (2nd order differencing is used across the boundaries). When the temperature structure is solved for in an implicit time-dependant manner (as we do) this ap-
proach is numerically stable. Thus, our calculation of the flaring angle is local in the sense that changes in surface density, opacity or temperature affect the flaring angle at that position. However, as we shall discuss in Section 5.2 our method does not allow for shadowing, which as we shall see, should occur in these discs. Equation 31 is solved implicitly using the LSODA numerical library for ODEs found in ODEPACK (Hindmarsh 1983). We choose a relative tolerance for the implicit solver of $10^{-5}$ which provides a good balance between speed and accuracy.

4.4 Boundary conditions and numerical grid

We are only interested in the physics of the snow-lines in the outer regions of the protoplanetary discs. However, truncating the grid inward of several AU results in an issue. In order to calculate the temperature outward of the inner boundary we need to know the temperature ($\gamma$) inside the inner boundary. Simply guessing this temperature results in unphysical solution. Instead, if we pick our inner boundary to be on sub-AU scales, then the disc is in the flat-disc heating approximation, where the finite size of the star dominates the flux absorbed by the disc (the first term in Equation 10). In this limit $\gamma$ is known analytically to be $1.125$ (Chiang & Goldreich 1997). Therefore we chose our inner boundary to be at 0.04 AU. Setting $\gamma = 1.125$ at the boundary allows us to solve for the temperature structure of the entire disc. Finally, $\gamma$ is chosen to be constant across the outer boundary.

The large dynamical range in scales necessitates a logarithmic grid. We use 550 cells with an outer boundary of 300 AU. At the inner boundaries we use an outflow boundary condition for all the species and the radial radiative flux is set to zero. At the outer boundaries the particle size is set to be in drift-growth equilibrium for a $T_m \propto R^{-1/2}$ temperature profile. For the radial radiative diffusion term, $H/R$ is assumed to be constant across the boundary.

Our requirement to include the inner disc for the temperature calculation causes in two issues that produce small time-steps. Firstly the small grid cells and large particle sizes that can be reached in the inner disc due to continued growth (as we have not included fragmentation in our size evolution model), produce rapid drift with short time-steps. To mitigate this, once the dust size has grown to 5 cm it cannot grow further (this happens inside a few AU where the disc is optically thick and therefore insensitive to the actual particle size). Further, the small cell sizes in the inner disc result in short viscous timescales and consequently short time-steps. To mitigate this, inside an AU we smoothly reduce the viscosity by two orders of magnitude. Again as the disc is optically thick this has no effect on our calculations, and we note again the gas profile is fixed and does not evolve. With these choices the time-step allows manageable computations over Myr timescales, but still includes the full disc for the radiative transfer calculation.

We note the inclusion of the radiative diffusion term acts to also numerically stabilise the scheme.

4.5 Results

As expected at intermediate optical depths, we find that the CO snow-line is thermally unstable and evolves through a limit-cycle where parts of the disc periodically condense and sublimate. Perhaps one of the most extraordinary findings is the scale over which this can happen. We find the CO snow-line can move 10s of AU! We find this behaviour to be robust to choices of opacity-laws, viscosity, disc properties and numerical parameters. We run all our simulations for several Myr and find that they do not relax to a steady-state, rather they enter a regime where they repeatedly evolve through a limit-cycle.

Working with our simple opacity law (Equation 20), we consider our standard model to be a 0.035 M$_\odot$ gas disc where the outer regions have been depleted slightly, so that the dust-to-gas ratio at 300 AU is 1/300 (note the dust-to-gas ratio typically increases inwards). We choose a viscous alpha of $10^{-3}$ and assume that at the outer boundary 20% of the total solid’s mass is in CO ice (disc evolution calculations based on static chemistry put this value in the range 20-50%, e.g. Madhusudhan et al. 2014). In Figure 5, we show snapshots of the solid surface density as a function of time. This figure indicates that the snow-line advances from $\sim 55$ AU to $\sim 30$ AU over a timescale of order 1000 years. It then spends several thousands to 10s of thousands of years with the snow-line at $\sim 30$ AU before retreating back to $\sim 55$ AU on a timescale of 1000 years. During this time the solid-surface density in the region of 30-50 AU increases by an order of magnitude.

This rapid increase in solid surface density is easy to understand by looking at Figure 6 where we plot the temperature and maximum particle size as well as the solid surface density, solid surface density excluding CO ice and CO vapour surface density. The three columns show these quantities before the snow-line rapidly moving inwards (left), while it is moving inwards (middle) and while it is moving outwards (right). The CO vapour density rapidly increases inside the snow-line. This is well known (e.g. Stevenson & Lunine 1988), as the dust drifts rapidly with respect to the gas, once the CO sublimes it moves much more slowly at the gas velocity. Thus, mass-conservation requires a much higher surface density. Once the snow-line moves it progressively condenses the CO vapour resulting in high solid densities.

One of the intriguing consequences is the solid surface density changes inwards of the snow-line (around 20 AU) in the top panels of Figure 6. The consequence of these perturbations can be understood by looking at the evolution of the mid-plane temperature. As the snow-line moves inwards it flattens the temperature profile in the vicinity of the snow-line (middle panel of Figure 6). A flatter temperature profile creates a weaker mid-plane pressure gradient and slow solid drift velocities. Thus, CO-ice free solids pile-up at the snow-line creating a density perturbation that then drifts inwards once the snow-line recedes and the drift speed increases. Dust diffusion smears out the density bumps as they drift inwards, but they can still be seen inwards of 10 AU, with, in some cases, order unity changes in the dust surface density. Therefore, not only do you get solid surface-density perturbations at the snow-line, but also perturbations at smaller radii that were created by previous movement of the
Snow-lines can be thermally unstable

Figure 5. Snapshots of the solid (CO ice + non CO ice) surface density as a function of time. The left panel shows the snow-line advancing inwards. The right panel shows the snow-line retreating outwards.

Figure 6. The top row shows the solid surface density, solid surface density excluding CO ice and CO vapour surface density. The middle and bottom rows show the mid-plane temperature and maximum particle sizes respectively. The left column shows the disc before the snow-line starts to rapidly move inwards, the middle shows the snow-line while it is moving inwards rapidly and the right shows while it is moving outwards. The horizontal band in the temperature panel shows the range of temperatures over which the ice fraction changes significantly and is representative of the CO sublimation temperature.
Figure 7. The evolution of the disc at 50 AU in the CO surface density – mass-flux plane. The line traces out the limit cycle performed by this patch of the disc over one cycle. The overall cycle takes approximately 70,000 years. The colour of the points map the time evolution, where the bottom-left of the cycle is defined to have zero time. The dashed line indicates the CO mass flux at which the disc is being fed at the outer boundary.

Figure 8. The evolution of the snow-line (taken to be the location where $X_{\text{CO}} = 0.5$) position as a function of time. While individual snow-line evolutions are all slightly different the overall pattern is regularly repeated, with a cycle length of $\sim 70$ kyr.

snow-line. We find this effect is more pronounced at higher dust-to-gas ratios and CO-ice fractions (see Figure 10).

Finally, the bottom row of Figure 6 also shows the maximum particle size is only marginally affected by the change in solid surface density and movement of the snow-line. This is primarily because the change in surface density and movement of the snow-line is comparable or shorter in timescale to the growth timescale.

We can investigate how well our simple picture developed previously works in practice by plotting how our numerical model traverses the CO surface density and CO mass-flux plane. In Figure 7 we plot the actual limit-cycle the disc performs at 50 AU. The limit cycle looks qualitatively similar to those shown in Figure 4. The CO mass-flux at which the disc is being fed lies in the forbidden region of the S-curve. The evolution around the limit-cycle indicates that the 50 AU annulus spends the majority of it’s time ($\sim 50$ kyr), in the vapour phase and the rest in the solid phase. Therefore, the duty cycle for this set of parameters, is such that the snow-line spends the largest fraction of it’s time at larger radii, before propagating inwards and spending a smaller fraction of its time at closer orbital distances. This is shown in Figure 8 where we plot the snow-line position as a function of time.

The narrow range of CO surface densities which the limit-cycle traverses is indicative of the steepness of the mid-plane temperature profile ($\frac{\text{d} \log T_{\text{mid}}}{\text{d} \log R} \sim -0.5 - 0.6$), where steeper temperature gradients give rise to smaller dynamic ranges in the limit cycle (Figure 4). We cannot compare our numerical evolutionary calculations to any steady-state S-curve, as the background temperature profile evolves throughout the evolution of the disc (middle-panels of Figure 6). Further, we note that that the disc does not perform a perfect limit-cycle. The bottom-left of Figure 7 indicates that once the CO sublimes into the CO vapour phase (the drop from high CO mass fluxes to low) the disc then evolves to lower CO surface densities, before then evolving to high CO surface densities as expected. This behaviour is generic, and is driven by diffusion. Once the CO locally sublimes into the vapour phase there is an over-concentration of CO vapour which diffuses away, lowering the CO surface density.

4.5.1 Small parameter exploration

The parameter space to explore for this new thermal instability is vast, even if we restricts ourselves to just the CO snow-line. Here we only explore the dependence of several key parameters.

Firstly, our understanding of the thermal instability is that if we move to low or high optical depths then the snow-line would indeed be thermally stable. We can modify the optical depth at the snow-line by changing the dust-to-gas ratio at the outer boundary. In the case of our nominal model the optical depth while CO is in the vapour phase is $\sim 0.1$ and $\sim 0.8$ when CO is in the solid phase. Therefore, changing the dust-to-gas ratio at the outer boundary to values of 1/2000 and 1/30 we find stable, time-invariant snow-lines occurring around 50-60 AU.

Next we consider how changing the dust-to-gas ratio, the viscous alpha and the CO ice fraction controls the snow-line behaviour. The evolution of the snow-line radius as a function of time is shown in Figure 9 where the dust-to-gas ratio, viscosity and CO ice fraction are modified. The evolution of these different parameters can be compared to our nominal model shown in Figure 8.

Due to the steep concentration gradients that occur at the snow-line, the primary driver, and the easiest way to understand the effect of changing disc conditions, is diffusive transport across the snow-line. Larger concentration gradients, or higher values of the viscosity result in higher radial diffusive fluxes across the snow-line and faster evolution. Therefore, higher viscosities result in faster evolution around the limit-cycle while its properties are generally preserved (bottom three panels of Figure 9). The higher CO mass-fraction between the third panel in Figure 9 and the nominal case (Figure 5) similarly results in faster evolution around the limit-cycle due to the higher concentration gradients formed.

Finally, the changes due to the dust-to-gas ratio can also be understood mainly in terms of radial transport across the snow-line (factors like the thermal timescale play a minor role). Higher dust-to-gas ratios result in faster particle
Snow-lines can be thermally unstable

4.5.2 More physically motivated opacity laws

In much of the previous analysis we have used a very simple opacity law that does not depend on the maximum particle size (Equation 20). However, the opacity does vary with maximum particle size. Here we show results for opacity laws motivated from geometric optics (Equation 21) where the Rayleigh index ($\beta$) is varied. Silicate grains have $\beta \sim 2$, whereas water-ice-silicate mixtures have lower values of $\beta$ (e.g. Chiang et al. 2001). In Figure 11, we show the snow-line evolution as a function of time for $\beta$ values of 1 and 2.

This figure shows the evolution of the snow-line is faster and occurs over a smaller radial range than the cases with the simple opacity law. The changes are not explicitly due to the differences in opacities themselves, but rather the effect they have on the dust-to-gas ratio and particle size. The modified opacities tend to result in steeper disc temperature gradients (hence a narrower radial range over which a snow-line can exist), and higher dust-to-gas ratios in the vicinity of the snow-line. Hence the snow-line evolution is faster, analogous to those models with higher dust-to-gas ratios with the nominal opacity (c.f. top panel Figure 9).
5 DISCUSSION

In this work we have shown that snow-lines in the outer regions (moderate optical depths) of protoplanetary discs are subject to thermal instabilities. The fact that the thermal instability only exists at moderate optical depths probably means that it will not affect the water snow-line under standard conditions. However, it is likely to control the dynamics of many other snow-lines that occur at cooler temperatures (e.g. carbon monoxide, carbon dioxide, ammonia etc.).

In the context of protoplanetary discs this thermal instability results in a limit-cycle where volatiles in the disc progressively sublimate and then condense. In keeping with other accretion disc thermal instabilities this limit-cycle can be analysed in the context of an “S-curve”, where there is a forbidden range of mass-fluxes. The simulations also indicate evolution occurring for higher viscosities, CO ice-mass fraction of the CO snow-line can vary significantly, with faster standard conditions. However, it is likely to control the dynamics of many other snow-lines that occur at cooler temperatures (e.g. carbon monoxide, carbon dioxide, ammonia etc). Secular instabilities (i.e. instabilities that exist in the standard thin disc accretion models), such as our snow-line thermal instability, have a long history, and their true nature has been extensively debated (as early as, e.g. Pringle 1981). It is important to realise they are not “real” instabilities in the standard hydrodynamical sense. Therefore, it remains an open question as to how this thermal instability (and others) behave in real hydrodynamic discs. While there has been some success in recovering S-curve-like evolution in hydrodynamic models for other thermal instabilities (e.g. dwarf nova outbursts, Coleman et al. 2016), these are not applicable to our snow-line thermal instability. For example, since we have temperature changes in our discs how do these affect the hydrodynamics of the underlying disc? Further, we note that the thermal timescales of the outer regions of protoplanetary discs can be fairly short, even comparable to the dynamical timescale (∼ 1/Ω_k). Therefore, while we have assumed that the disc is in vertical hydrostatic equilibrium throughout our models (this is one of the basic assumptions of the thin disc model), this response may not be as instantaneous as we have assumed. Further, as discussed in section 4.1.1 we have not considered what happens if the viscosity changes due to the temperature changes, which would cause the gas disc to evolve. Nor have we included the dynamical feedback of the dust on the gas, which would also increase the richness of the problem. However, we end on a note of optimism: our calculations have shown that whatever happens, snow-lines are not stable structures and should evolve.

5.1 Limitations

We add several notes of caution to our work. This work has all been performed in a 1D model, where mid-plane values are taken to be representative of the disc. It is well known that snow-lines are two dimensional structures (e.g. Min et al. 2011; Qi et al. 2019), and vertical mixing of both volatiles and solids are important (Krijt et al. 2018), and may qualitatively change our results. Since the majority of the mass is contained near the mid-planes of thin discs, we suspect our model does capture the basic physics, and it is unclear how 2D effects could stabilise a snow-line against this thermal instability.

Further, we have implicitly assumed that the dust temperature is instantaneously transferred to the gas. In reality this change takes place over a finite time. This could potentially slow the evolution of our thermal instability.

Finally, since we have assumed that the disc is being fed at a steady rate the rise in CO vapour surface density inside the snow-line extends all the way to the inner disc. Disc evolution models tend to find the CO vapour density is enhanced interior to the snow-line in a ring, rather than a continuous increase (e.g. Booth et al. 2017). This may mean that the very high increase in ice mass, that occurs as the snow-line propagates inwards by 10s of AU, is overestimated.

5.1.1 Are secular instabilities captured by secular models?

Secular instabilities (i.e. instabilities that exist in the standard thin disc accretion models), such as our snow-line thermal instability, have a long history, and their true nature has been extensively debated (as early as, e.g. Pringle 1981). It is important to realise they are not “real” instabilities in the standard hydrodynamical sense. Therefore, it remains an open question as to how this thermal instability (and others) behave in real hydrodynamic discs. While there has been some success in recovering S-curve-like evolution in hydrodynamic models for other thermal instabilities (e.g. dwarf nova outbursts, Coleman et al. 2016), these are not applicable to our snow-line thermal instability. For example, since we have temperature changes in our discs how do these affect the hydrodynamics of the underlying disc? Further, we note that the thermal timescales of the outer regions of protoplanetary discs can be fairly short, even comparable to the dynamical timescale (∼ 1/Ω_k). Therefore, while we have assumed that the disc is in vertical hydrostatic equilibrium throughout our models (this is one of the basic assumptions of the thin disc model), this response may not be as instantaneous as we have assumed. Further, as discussed in section 4.1.1 we have not considered what happens if the viscosity changes due to the temperature changes, which would cause the gas disc to evolve. Nor have we included the dynamical feedback of the dust on the gas, which would also increase the richness of the problem. However, we end on a note of optimism: our calculations have shown that whatever happens, snow-lines are not stable structures and should evolve.

5.2 Shadowing

As discussed when we set-up our radiative transfer scheme, we are unable to include the effects of shadowing. Specifically, if the height of the photosphere blocks stellar light at more distant radii our model will not capture this. Since the evolving snow-line results in local surface density changes shadows are cast. As we are explicitly calculating the height of the photosphere, we can check whether our disc would have cast shadows.

We identify two types of shadow: firstly, shadows cast by the rapid increase in dust surface density exterior to the snow-line; secondly, the surface density perturbations that the moving snow-line creates in the down-stream dust surface density profile (Figure 10) can also cast shadows. We show both these types of shadows in Figure 12 computed from snapshots of our “nominal” case.

MNRAS 000, 1–16 (2015)
Shadowing will result in a temperature minimum in the disc; similar to shadowing from the inner rim at the dust sublimation front (Dullemond et al. 2001), where the heating comes from the radial radiative flux and scattering. Therefore, in addition to the snow-line-created surface density structure, we speculate that these surface density structures will create further surface density structures due to pressure trapping and expulsion. Thus, there is potential that snow-lines can create many, time-variable, surface density structures. However, in order to make progress we either need to find a way of including shadows in our simple 1D radiative transfer scheme (something that has proved difficult in the past - e.g. Dullemond 2000), or move to a 2D radiative transfer scheme, although it must be non-grey.

5.3 Observations of ringed discs

Since the original high-resolution ALMA observation of HL Tau (ALMA Partnership et al. 2015) there have been many observations of protoplanetary discs showing ringed substructure (e.g. Isella et al. 2016; Fedele et al. 2018; Andrews et al. 2018; Andrews 2020). While the community appears to favour a planetary origin for these structures (e.g. Zhang et al. 2018), surface-density perturbations arising from snowlines was among the ideas originally proposed (Zhang et al. 2015; Okuzumi et al. 2016). Recent work by Huang et al. (2018) and van der Marel et al. (2019) has suggested that snow-lines cannot be the cause, since the observed structures do not appear to show preferred radial spacing ratios. Such preferred radial spacing ratios would be expected if discs had fixed radial temperature profiles (e.g. $T \propto R^{-1/2}$) and snow-lines occurred at a set temperature.

We have shown snow-lines evolve in time and do not occur at fixed radial locations (especially in the outer regions of protoplanetary discs covered by the ALMA observations). Thus, such simple comparisons of radius ratios cannot be used to disprove or test the snow-line scenario. Further, even our simulations without shadowing show multiple, time-dependent structures from a single snow-line. The inclusion of shadowing is only likely to increase the number of ring-like structures arising from snow-lines. Therefore, while there is still much work to be performed, we speculate that the ALMA ringed discs could be caused by snow-line induced structures. Hence the observations are teaching us about chemistry and dust grain evolution in the outer regions of protoplanetary discs, rather than the properties of more mature planets.

6 CONCLUSIONS

Snow-lines are the regions where volatile species rapidly transition from the solid phase to the vapour phase and typically occur in the outer regions of protoplanetary discs. The outer regions of protoplanetary discs are passively heated by re-radiated stellar light from the disc’s surface. The absorption of this re-radiated stellar light is primarily done by the solids. Since the temperature profile controls the position of the snow-line, and the position of the snow-line controls the temperature (through the distribution of solids), the radiative properties and chemistry of protoplanetary discs are inextricably linked. In this work, we have studied this coupling both analytically and numerically, indicating snow-lines can be thermally unstable. Our main conclusions are summarised below:

(i) Snow-lines are thermally unstable at intermediate optical depths ($\tau \sim 0.05$ – 2). Therefore, many common snowlines (CO, CO$_2$, NH$_3$, N$_2$) cannot exist at fixed radial locations and must evolve in time. As the water snow-line is at high optical depths ($\tau \gg 1$, and viscously heated) in standard protoplanetary discs it is likely to be thermally stable.

(ii) The unstable snow-lines evolve through a limit-cycle, where patches of the disc spend some of their time at cool temperatures, with the volatile species in the ice phase and some of their time at high temperatures, with the volatile species in the vapour phase.

(iii) This limit-cycle can be understood in terms of an S-curve, by an analogy to other accretion disc thermal instabilities.

(iv) Numerical models that explicitly couple the temperature structure to the distribution of solids using a non-grey radiative transfer scheme show the CO snow-line moves over 10s of AU on $\sim 1,000$ – 10,000 year timescales.

(v) The evolving snow-line creates ring-like structures interior to the snow-line that may be the origin of the observed ALMA structures.

While we have shown this snow-line thermal instability to be robust, the simplicity of our numerical model requires more work in the future. Priorities for future work are investigating the role of shadows cast by the time-evolving snow-line and investigating the 2D nature of the problem.
ACKNOWLEDGEMENTS

I thank the referee for comments which improved the manuscript. JEO is supported by a Royal Society University Research Fellowship. I’m grateful to Doug Lin for suggesting that the role of latent heat should be explored. I also thank Richard Booth, Ruth Murray-Clay and Giovanni Rosotti for useful discussions.

REFERENCES

ALMA Partnership et al., 2015, ApJ, 808, L3
Aikawa Y., Miyama S. M., Nakano T., Umebayashi T., 1996, ApJ, 467, 684
Andrews S. M., 2020, arXiv e-prints, p. arXiv:2001.05007
Andrews S. M., et al., 2018, ApJ, 869, L41
Armitage P. J., Livio M., Pringle J. E., 2001, MNRAS, 324, 705
Bai X.-N., Stone J. M., 2013, ApJ, 769, 76
Bai X.-N., Ye J., Goodman J., Yuan F., 2016, ApJ, 818, 152
Bergin E. A., Williams J. P., 2018, arXiv e-prints, p. arXiv:1807.09631
Bergin E. A., et al., 2013, Nature, 493, 644
Birnstiel T., Dullemond C. P., Brauer F., 2010, A&A, 513, A79
Birnstiel T., Andrews S. M., Ercolano B., 2012, A&A, 544, A79
Bitsch B., Crida A., Morbidelli A., Kley W., Dobbs-Dixon I., 2013, A&A, 549, A124
Booth R. A., Ilee J. D., 2019, MNRAS, 487, 3998
Booth R. A., Owen J. E., 2020, MNRAS, 493, 5079
Booth R. A., Clarke C. J., Madhusudhan N., Ilee J. D., 2017, MNRAS, 469, 3994
Brauer F., Dullemond C. P., Henning T., 2008, A&A, 480, 859
Cannizzo J. K., 1993, ApJ, 419, 318
Chiang E. I., Goldreich P., 1997, ApJ, 500, 411
Chiang E. I., Joung M. K., Creech-Eakman M., Qi C., Kessler J. E., Blake G. A., van Dishoeck E. F., 2001, ApJ, 547, 1077
Coleman M. S. B., Kotko I., Blaes O., Lasota J. P., Hirose S., 2016, MNRAS, 462, 3710
Cuzzi J. N., Zahnle K. J., 2004, ApJ, 614, 490
D’Alessio P., Cantó J., Calvet N., Lizzano S., 1998, ApJ, 500, 411
D’Alessio P., Calvet N., Hartmann L., 2001, ApJ, 553, 321
Dullemond C. P., 2000, A&A, 361, L17
Dullemond C. P., Natta A., 2003, A&A, 405, 597
Dullemond C. P., Dominik C., Natta A., 2001, ApJ, 560, 957
Faulkner J., Lin D. N. C., Papaloizou J., 1983, MNRAS, 205, 359
Fedele D., et al., 2018, A&A, 610, A24
Gressel O., Turner N. J., Nelson R. P., McNally C. P., 2015, ApJ, 801, 84
Guidi G., et al., 2016, A&A, 588, A112
Hayashi C., 1981, Progress of Theoretical Physics Supplement, 70, 35
Hindmarsh A. C., 1983, Scientific Computing, pp 55–64
Hollenbach D., Kaufman M. J., Bergin E. A., Melnick G. J., 2009, ApJ, 690, 1497
Huang J., et al., 2018, ApJ, 869, L42
Isella A., et al., 2016, Phys. Rev. Lett., 117, 251101
Kama M., et al., 2020, A&A, 634, A88
Kretke K. A., Lin D. N. C., 2007, ApJ, 664, L55
Krijt S., Schwarz K. R., Bergin E. A., Ciesla F. J., 2018, ApJ, 864, 78
Kuiper R., Klahr H., Dullemond C., Kley W., Henning T., 2010, A&A, 511, A81
Lasota J.-P., 2001, New Astron. Rev., 45, 449
Madhusudhan N., Amin M. A., Kennedy G. M., 2014, ApJ, 794, L12
Martin R. G., Livio M., 2012, MNRAS, 425, L6
Martin R. G., Livio M., 2014, ApJ, 783, L28
Martin R. G., Lubow S. H., 2011, ApJ, 740, L6

This paper has been typeset from a TeX/LaTeX file prepared by the author.