ON THE EVOLUTION OF THE CO SNOW LINE IN PROTOPLANETARY DISKS

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ABSTRACT

CO is thought to be a vital building block for prebiotic molecules that are necessary for life. Thus, understanding where CO existed in a solid phase within the solar nebula is important for understanding the origin of life. We model the evolution of the CO snow line in a protoplanetary disk. We find that the current observed location of the CO snow line in our solar system, and in the solar system analog TW Hydra, cannot be explained by a fully turbulent disk model. With time-dependent disk models we find that the inclusion of a dead zone (a region of low turbulence) can resolve this problem. Furthermore, we obtain a fully analytic solution for the CO snow line radius for late disk evolutionary times. This will be useful for future observational attempts to characterize the demographics and predict the composition and habitability of exoplanets.

Key words: accretion, accretion disks – planets and satellites: formation – protoplanetary disks – stars: pre-main sequence

1. INTRODUCTION

The most abundant volatiles in a protoplanetary disk are CO, CO\textsubscript{2}, and H\textsubscript{2}O. A snow line marks a radial location in a disk where the mid-plane temperature\textsuperscript{4} drops sufficiently so that a volatile condenses out of the gas phase to become solid.\textsuperscript{5} Thus, each volatile has a different snow line radius, water ice being closest to the host star, then CO\textsubscript{2} and then CO. Snow lines are thought to regulate the planet formation process (e.g., Öberg et al. 2011). Giant planets, for instance, are expected to form outside the water snow line because the density of solids is significantly higher outside of this radius (e.g., Pollack et al. 1996; Morales et al. 2011; Ros & Johansen 2013). Snow lines are also important because dust piles up in the pressure trap just inside the snow line and the grains become stickier as ice condenses on their surfaces. The composition of a planet and its atmosphere are determined by where the planet forms, and where it accretes material relative to the snow lines (e.g., Öberg et al. 2011).

The water snow line occurs at a temperature of around 170 K (Hayashi 1981) and currently in our solar system is observed to be at a radius of 2.7 AU, within the asteroid belt (Abe et al. 2000; Morbidelli et al. 2000; Martin & Livio 2013b). The CO snow line occurs at a cooler temperature of about $T_{\text{CO,snow}} = 17$ K (Öberg et al. 2005). Comets from the Kuiper belt have varying amounts of CO, suggesting that they formed close to the CO snow line (A’Hearn et al. 2012). Some dwarf planets such as Pluto and comets in the Kuiper belt contain the even more volatile N\textsubscript{2} gas (e.g., Cochran et al. 2000) implying that they may have formed beyond the CO snow line. The Kuiper belt is currently thought to have formed in the approximate region 27–35 AU (Levison et al. 2008) and thus, at the time of planetesimal formation the CO snow line would have been in this region. The CO snow line could mark the transition from the planet forming region to the formation of smaller icy bodies and dwarf planets, like Pluto.

The water snow line is hard to observe in exosolar systems because it is very close to the star. However, the CO snow line is an easier target because it is farther away. The best studied CO snow line is in a solar nebula analog disk around TW Hya. The star has a mass of $0.8 M_\odot$ and an age of less than 10 Myr (Hoff et al. 1998). Qi et al. (2013) observed the reactive ion N\textsubscript{2}H\textsuperscript{+} which is only present where CO is frozen out. They found that the CO snow line lies at 28–31 AU, similar to that in our solar system.

Understanding the evolution of the CO snow line is essential to deciphering the origins of prebiotic molecules that are necessary for life (Tielens & Charnley 1997). CO ice is needed to form methanol which is a building block for more complex organic molecules. Comets are thought to have bombarded the early Earth, thus delivering these molecules to Earth and allowing life to emerge. In this work we therefore consider the evolution of the CO snow line in various models of protoplanetary disks.

Angular momentum transport in protoplanetary disks is thought to be driven by turbulence generated by the magnetorotational instability (MRI; Balbus & Hawley 1991). However, it is now widely acknowledged that protoplanetary disks are not sufficiently ionized for the MRI to operate throughout. They contain a dead zone, a region of low turbulence at the disk mid-plane where the MRI is suppressed (e.g., Gammie 1996). In the present Letter, we investigate the evolution of the CO snow line in disks with and without a dead zone.

2. FULLY MRI TURBULENT DISK MODEL

Material in an accretion disk orbits the central mass, $M_*$, with Keplerian velocity at radius $R$ with angular velocity $\Omega = \sqrt{GM_*/R^3}$ (e.g., Lynden-Bell & Pringle 1974; Pringle 1981). The viscosity in a fully MRI turbulent disk may be parameterized with

$$\nu = \alpha_m \frac{c_s^2}{\Omega},$$

where the Shakura & Sunyaev (1973) viscosity parameter is $\alpha_m$, the sound speed is $c_s = \sqrt{RT_\text{c}/\mu}$, $R$ is the gas constant, $\mu$ is the gas mean molecular weight and $T_\text{c}$ is the mid-plane temperature.
is found from the radius of the star. The mid-plane temperature of the disk is 

\[ T = \frac{\alpha M}{3\pi} \]

(Pringle 1981), where the infall accretion rate is \( M \) and is constant through all radii. The surface temperature in the steady disk is

\[ \sigma T_s^4 = \frac{9}{8} \frac{M}{3\pi} \Omega^2 + \sigma T_{\text{irr}}^4 \]

(e.g., Cannizzo 1993; Pringle et al. 1986). For an unflared disk, the irradiation temperature is

\[ T_{\text{irr}} = \left( \frac{2}{3\pi} \right)^{1 \over 4} \left( \frac{R_s}{R} \right)^{1 \over 2} T_s \]

(Chiang & Goldreich 1997), where \( T_s \) is the temperature and \( R_s \) is the radius of the star. The mid-plane temperature of the disk is found from

\[ T_s^4 = \tau T_{\text{e}}^4 \]

where the optical depth is

\[ \tau = \frac{3}{8} \frac{\Sigma}{\kappa} \]

and the opacity is

\[ \kappa = a T_{\text{e}}^b. \]

Dust dominates the absorption properties of matter where it is present. Thus, for the low temperatures close to the CO snow line, we take \( a = 0.053 \) and \( b = 0.74 \) (see Zhu et al. 2009 and also Bell & Lin 1994). However, we note that the exact values do not affect the disk temperature strongly (see Equation (5)).

We solve the equation \( T_{\text{e}} = T_{\text{CO, snow}} \) to find the CO snow line radius, \( R_{\text{CO, snow}} \). This radius is shown in Figure 1 by the short-dashed line as a function of the accretion rate, \( M \), for \( M_* = 1 M_\odot \), \( \alpha_m = 0.01 \), \( T_{\text{CO, snow}} = 17 K \), \( T_* = 4000 K \), and \( R_* = 3 R_\odot \). Because the accretion rate through the disk drops in time, time is the implicit coordinate here. There is still some uncertainty concerning the value for \( \alpha_m \) in protoplanetary disks (e.g., King et al. 2007) and thus we also show a disk model with a small \( \alpha_m = 10^{-4} \) by the long-dashed line. Given that the CO snow line in our solar system is thought to have been in the range 27–35 AU at the time of planetesimal formation, the CO snow line appears to have the same evolution problems as the water snow line (Garaud & Lin 2007; Oka et al. 2011; Martin & Livio 2012). That is, in a fully MRI turbulent disk, the CO snow line moves in too close to the host star during the low accretion rate phase toward the end of the disk lifetime. Thus, in the following section we consider a time-dependent disk with a dead zone in order to track the evolution of the CO snow line in a more realistic disk model.

For comparison to water snow line models, we find an analytic fit to the CO snow line radius. On scales of tens of AU, the irradiation is certainly the dominant heating source. Thus, we find an approximate analytical steady state solution by ignoring the viscous heating term in Equation (3) so that \( T_{\text{e}} = T_{\text{irr}} \). In this limit

\[
R_{\text{CO, snow}} \approx 13.2 \left( \frac{\alpha_m}{0.01} \right)^{-1/7} \left( \frac{M_*}{M_\odot} \right)^{1/7} \left( \frac{M}{10^{-8} M_\odot \text{yr}^{-1}} \right)^{1/7} \times \left( \frac{T_{\text{CO, snow}}}{17 K} \right)^{-0.95} \left( \frac{R_*}{3 R_\odot} \right)^{1/7} \left( \frac{T_*}{4000 K} \right)^{1/7} \text{AU.}
\]

(8)

This is almost identical to the full solution shown in the dashed lines in Figure 1 for accretion rates \( M \lesssim 10^{-8} M_\odot \text{yr}^{-1} \), where irradiation dominates the viscous heating term. For higher accretion rates, this formula underestimates the CO snow line radius.

3. A DISK WITH A DEAD ZONE

When the ionization fraction is not sufficiently high for the MRI to drive turbulence, a dead zone forms (see disk structure sketches in Martin & Livio 2013a). The hot inner parts of the disk with mid-plane temperature \( T_{\text{e}} > T_{\text{crit}} \) are thermally ionized and thus MRI active. The value of \( T_{\text{crit}} \) is thought to be around 800 K (Umebayashi & Nakano 1988). Farther away from the central star, cosmic rays or X-rays from the star are the dominant source of ionization (Glassgold et al. 2004) and these can only penetrate the surface layers with surface density \( \lesssim \Sigma_{\text{crit}} \). Where the total surface density, \( \Sigma \), is larger than this critical value, \( \Sigma > \Sigma_{\text{crit}} \), a dead zone exists at the mid-plane with surface density \( \Sigma_{\text{e}} = \Sigma - \Sigma_{\text{crit}} \). Thus, the MRI is only active in the surface layers. The precise value of \( \Sigma_{\text{crit}} \) remains uncertain (e.g., Martin et al. 2012a, 2012b). If cosmic rays are the dominant ionization source, it may be as high as \( \Sigma_{\text{crit}} = 200 \text{ g cm}^{-2} \) (Gammie 1996; Fromang et al. 2002) but if X-rays dominate the active layer is much smaller (Matsumura & Pudritz 2003). In the outer parts of the disk, where \( \Sigma < \Sigma_{\text{crit}} \), the external ionization sources penetrate to the mid-plane and the disk is fully MRI active. In all parts of the disk that are MRI active, we assume the same constant viscosity parameter, \( \alpha_m \).

Build up of material within the dead zone may cause the disk to become self gravitating. This occurs when the Toomre (1964)
parameter, \( Q = c_s \Omega / \pi G \Sigma \), drops below its critical value that we take to be \( Q_{\text{crit}} = 2 \). A second type of turbulence, gravitational turbulence, is driven with viscosity

\[
v_g = \alpha_g \frac{c^2}{\Omega}.
\]

We take the Shakura & Sunyaev (1973) parameter to be

\[
\alpha_g = \alpha_m \exp(-Q^4)
\]

(e.g., Zhu et al. 2010a). However, providing that the function decreases strongly with \( Q \), the form does not significantly affect the viscosity (Zhu et al. 2010a, 2010b; Martin & Lubow 2013).

In this section we first consider time-dependent numerical models of a disk with a dead zone and then we find analytic approximations to the CO snow line radius in such a model.

### 3.1. Time-dependent Protoplanetary Disk Models

We consider a model for the collapse of a molecular cloud on to the disk (Armitage et al. 2001; Martin et al. 2012b). Initially the accretion rate on to the disk is \( 2 \times 10^{-6} M_\odot \text{yr}^{-1} \) and this decreases exponentially on a timescale of \( 10^5 \) yr. The initial surface density of the disk is that of a fully turbulent steady disk with an accretion rate of \( 2 \times 10^{-6} M_\odot \text{yr}^{-1} \) around a star of mass \( M_* = 1 M_\odot \). We take a radial grid of 200 points evenly distributed in \( \log R \) from \( R = 1 \) AU up to \( R = 200 \) AU and infalling material is added at a radius of \( R = 195 \) AU. The inner boundary has zero torque and the outer boundary has zero radial velocity. The CO snow line lies far from the inner edge of the disk. We take \( \alpha_m = 0.01 \) but note that the chosen value does not significantly affect the CO snow line evolution for the model with a dead zone. We consider two disk models, one that is fully MRI turbulent throughout and a second that has a dead zone determined by \( \Sigma_{\text{crit}} = 10 \text{g cm}^{-2} \). We solve the time-dependent accretion disk equations along with a simplified energy equation including viscous and irradiative heating terms (see Martin & Livio 2011, for more details). We chose \( T_* = 4000 \text{K}, R_* = 3 R_\odot \), and \( T_{\text{CO,snow}} = 17 \text{K} \).

The disk is gravito-magneto unstable for large infall accretion rates. This causes unsteady accretion on to the central star as the turbulence transitions from gravitationally produced to magnetically produced (Armitage et al. 2001; Zhu et al. 2009; Martin & Lubow 2011, 2013). In Figure 2 we show the evolution of the CO snow line as a function of time for the fully turbulent disk (dashed line) and the disk with a dead zone (solid line). The model with a dead zone has small and brief increases in the snow line radius which occur during the FU Orionis type outbursts. For later times (and smaller accretion rates), the disk with a dead zone has a CO snow line radius that is much larger than that of the fully turbulent disk model, and in agreement with that in our solar system. A dead zone therefore appears to be a necessary component in modeling protoplanetary disks.

With a dead zone included, we have shown that time-dependent numerical simulations predict a larger CO snow line radius (in agreement with the observations) because the small amount of self-gravity within the dead zone heats the more massive disk.

### 3.2. Analytical Solutions

We have shown in the previous section that the presence of a dead zone significantly affects the evolution of the CO snow line. Once the infall accretion rate drops sufficiently, the outbursts cease but a dead zone may still be present. Following

![Figure 2. Evolution of the CO snow line in a time-dependent disk with an exponentially decreasing infall accretion rate. The dashed line shows a fully MRI turbulent disk and the solid line a disk with a dead zone determined by \( \Sigma_{\text{crit}} = 10 \text{g cm}^{-2} \). The shaded region shows the location of the CO snow line in our solar system at the time of planetesimal formation.](image)

Martin & Livio (2013a), because the CO snow line is in the self-gravitating part of the dead zone, we find steady state analytic solutions for its radius. The solution has MRI active surface layers (with surface density \( \Sigma_{\text{crit}} \)) over a self-gravitating dead zone. In order to find analytic solutions, we work in the limit \( \Sigma \gg \Sigma_{\text{crit}} \) and approximate \( \Sigma_{\text{crit}} = 0 \).

When the disk is self-gravitating, it has surface density

\[
\Sigma = \frac{c_s \Omega}{\pi G Q}.
\]

For a steady state accretion disk the accretion rate is

\[
\dot{M} = 3 \pi v_g \Sigma.
\]

Both \( \Sigma \) and \( v_g \) depend on \( Q \), and thus we can relate the Toomre parameter to the accretion rate through

\[
\dot{M} = \left( \frac{3 c_s^2 \alpha_m}{G} \right) \exp(-Q^4) \frac{Q}{Q_{\text{crit}}}. \tag{13}
\]

The term in brackets is constant for a fixed CO snow line temperature. This expression depends sensitively on \( Q \) and thus for a reasonable range of accretion rates, \( Q \) is approximately constant (see also Martin & Livio 2012). We scale the variables to \( T_{\text{CO,snow}} = T_{\text{CO,snow}}/17 \text{K}, \alpha_m' = \alpha_m/0.01, M_*' = M_*/M_\odot, \) and \( R' = R/AU \) and solve Equation (13) to find the scaled Toomre parameter

\[
Q' = \frac{Q}{Q_{\text{crit}}} = 0.69 \left[ \frac{W(x)}{W(x_0)} \right]^{1/2}, \tag{14}
\]

where we define

\[
x = 2.45 \times 10^4 \frac{\alpha_m'^4 T_{\text{CO,snow}}^4}{M_*'^4}. \tag{15}
\]
and \( x_0 = 2.45 \times 10^7 \). The Lambert function, \( W \), is defined by the equation

\[
x = W(x) \exp[W(x)].
\]

The mid-plane temperature is related to the disk surface temperature through Equations (5)–(7). The steady energy equation is

\[
\sigma T^4_e = \frac{9}{8} \nu_c \Sigma \Omega^2 + \sigma T^4_{\text{in}}.
\]

We solve \( T_e = T_{\text{CO,snow}} \) to find the CO snow line radius and plot it as a function of the accretion rate. This is shown by the solid line in Figure 1 for \( M_* = 1 M_\odot \), \( T_{\text{CO,snow}} = 17 \) K, \( \alpha_m = 0.01 \), \( T_e = 4000 \) K, and \( R_e = 3 R_\odot \). The dashed lines are the fully turbulent disk model with \( \alpha_m = 0.01 \) (short-dashed) and \( \alpha_m = 10^{-4} \) (long-dashed). The solid line is the disk with a self-gravitating dead zone.

In the limit where the irradiation is the dominant heating source (for low accretion rates \( M \lesssim 10^{-8} M_\odot \text{ yr}^{-1} \)) we approximate Equation (17) with \( T_e = T_{\text{in}} \). This gives the analytic CO snow line radius

\[
R_{\text{CO,snow}} = 29.3 M_*^{\frac{3}{2}} R_*^{\frac{1}{2}} \nu_c^{\frac{3}{2}} T_e^{0.61} \frac{W(x)}{W(x_0)} \frac{1}{\pi} \text{AU}.
\]

Its value is given approximately by

\[
R_{\text{CO,snow}} \approx 29.3 \left( \frac{M_*}{M_\odot} \right)^{\frac{3}{2}} \left( \frac{R_*}{3 R_\odot} \right)^{\frac{1}{2}} \left( \frac{T_e}{4000 \text{ K}} \right)^{0.61} \left( \frac{T_{\text{CO,snow}}}{17 \text{ K}} \right)^{\frac{3}{2}} \times \left( \frac{M_\odot}{12 M_\odot} \right)^{\frac{1}{2}} \left( \frac{3 R_\odot}{R_\odot} \right)^{-\frac{1}{2}} \left( \frac{T_{\text{in}}}{4000 \text{ K}} \right)^{-0.61} \text{AU}.
\]

This is almost identical to the solid line shown in Figure 1 for low accretion rates. Note that this is independent of \( \alpha_m \).

In Figure 3 we show the surface density of the steady state solutions at the CO snow line radius (including both viscous and radiative heating terms). The disk with a dead zone has a fairly constant surface density at the snow line radius of around \( 100 \) g cm\(^{-2} \). Thus, provided that \( \Sigma_{\text{crit}} \ll 100 \) g cm\(^{-2} \), then the solutions presented in this section are valid. As shown in the previous section, \( \Sigma_{\text{crit}} = 10 \) g cm\(^{-2} \) was small enough for the dead zone to persist at the CO snow line radius for longer than the lifetime of the disk.

Submillimeter observations of TW Hya combined with radiative transfer calculations of the disk structure that assume a constant dust to gas ratio with radius predict a surface density about an order of magnitude lower than that required in our models (Andrews et al. 2012). However, their models were unable to reproduce both the brightness profiles and the CO line emission. It is possible that with the inclusion of a dead zone in their disk models that the observed features may be reproduced. The dead zone could explain why the dust emission has a sharp outer edge at \( 60 \) AU while the CO emission extends out past \( 215 \) AU and this should be investigated in future work.

4. DISCUSSION AND CONCLUSIONS

Shearing box simulations suggest that a small amount of turbulence may be driven in the dead zone by the turbulence in the disk surface layers (e.g., Fleming & Stone 2003; Simon et al. 2011). The addition of this small viscosity is unlikely to suppress outbursts (Martin & Lubow 2014), although the triggering may be due to heating from the additional turbulence, rather than self gravity (Bae et al. 2013). In the limit of small active layer surface density, the steady state dead zone solution would be the same as the fully MRI turbulent solution in Section 2 but with a smaller \( \alpha_m \). In the figures we have also considered a smaller turbulence of \( \alpha_m = 10^{-4} \) for this comparison. We find that, with an \( \alpha_m \), that is two orders of magnitude smaller than that in the active layers, it remains difficult to explain the current location of the CO snow line in our solar system, and in TW Hya.

The CO snow line in the disk around the Herbig Ae star HD 163296 has been found to lie at a radius of around \( 155 \) AU (Qi et al. 2011; Mathews et al. 2013). With observed parameters of \( M_* = 2.3 M_\odot \), \( T_e = 9333 \) K, \( R_e = 2 R_\odot \), and \( M = 7.6 \times 10^{-8} M_\odot \text{ yr}^{-1} \), our fully turbulent disk model (Equation (8)) predicts a CO snow line radius of \( 37 \) AU. The dead zone model (Equation (19)) predicts a radius of \( 62 \) AU. Thus, neither model can explain such a large CO snow line radius (although the model with a dead zone shifts the radius in the right direction). We suggest that disk flaring could account for this. Approximations for the temperatures of flared disks would predict a CO snow line radius \( > 100 \) AU (see Figure 4 in Chiang & Goldreich 1997). In contrast, the inner regions of the disk in TW Hya are flat, although it is moderately flared at radii \( R > 45 \) AU. Thus, flaring does not affect the CO snow line radius in TW Hya. Furthermore, this would suggest that our solar nebula was not flared, at least in the inner regions.

We have found that a fully MRI turbulent disk predicts a CO snow line that is much closer to the host star than that observed in our solar system and in the solar nebula analog TW Hya. With a dead zone, a small amount of self-gravity heats the more massive disk and the CO snow line radius is moved outward (in agreement with the observations). We have also found a fully analytic solution for the snow line radius in a disk with a dead zone for low infall accretion rates, appropriate for the later stages of protoplanetary disk evolution. The solution is valid providing that the surface density ionized by external
sources, \( \Sigma_{\text{crit}} \ll 100 \text{ g cm}^{-2} \). This formula could prove useful for determining composition and habitability of exosolar planets.

We thank an anonymous referee for comments that have improved the manuscript. R.G.M.’s support was provided under contract with the California Institute of Technology (Caltech) funded by NASA through the Sagan Fellowship Program.

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