Gas phase water in the surface layer of protoplanetary disks

C. Dominik\textsuperscript{1} C. Ceccarelli\textsuperscript{2} D. Hollenbach\textsuperscript{3} M. Kaufman\textsuperscript{3,4}

ABSTRACT

Recent observations of the ground state transition of HDO at 464 GHz towards the protoplanetary disk of DM Tau have detected the presence of water vapor in the regions just above the outer disk midplane (Ceccarelli et al. 2005). In the absence of non-thermal desorption processes, water should be almost entirely frozen onto the grain mantles and HDO undetectable. In this Letter we present a chemical model that explores the possibility that the icy mantles are photo-desorbed by FUV ($6 \text{ eV} \leq h\nu \leq 13.6 \text{ eV}$) photons. We show that the average Interstellar FUV field is enough to create a layer of water vapor above the disk midplane over the entire disk. Assuming a photo-desorption yield of $10^{-3}$, the water abundance in this layer is predicted to be $\sim 3 \times 10^{-7}$ and the average H$_2$O column density is $\sim 1.6 \times 10^{15} \text{ cm}^{-2}$. The predictions are very weakly dependent on the details of the model, like the incident FUV radiation field, and the gas density in the disk. Based on this model, we predict a gaseous HDO/H$_2$O ratio in DM Tau of $\sim 1\%$. In addition, we predict the ground state transition of water at 557 GHz to be undetectable with ODIN and/or HSO-HIFI.


1. Introduction

Water is a key ingredient in many astrophysical environments, including circumstellar disks. It is the main constituent of the icy mantles coating interstellar grains, and can
be one of the most abundant molecules in the gas phase. For these reasons, water may dominate both the chemistry (being a major oxygen reservoir) and the thermal balance (i.e. cooling) of the gas component of protostellar disks. In addition, water vapor and water ice in protoplanetary disks are the major reservoirs of water later to be found in planets, asteroids and comets and, therefore, are of great relevance for understanding the origin of the Solar System and the distribution of volatiles within it. Unfortunately, the observation of water molecules in interstellar space is nearly impossible from the ground because of the absorption by the terrestrial atmosphere. So far, just a handful of space-based instruments (ISO, SWAS and ODIN) have carried out observations of water vapor lines in interstellar molecular clouds, but these instruments did not have the sensitivity to observe water protoplanetary disks. However, the up-coming ESA/NASA mission Herschel will provide a sensitive instrument, HIFI, for these studies (Dominik & Ceccarelli 2005). Also, SOFIA has potential for water observations.

Meanwhile, HDO, as the most important isotope of water, is currently the best ground-based probe of the presence of water in astrophysical environments. Recently, Ceccarelli et al. (2005) reported the first discovery of HDO (and therefore also the first discovery of water) in a protoplanetary disk, namely DM Tau. The observations show an absorption line of gas phase HDO with a line-to-continuum ratio of 0.9 which translates into an average column density through the disk of $\sim 1.6 \times 10^{13}$ cm$^{-2}$. In the region where HDO is located, its fractional abundance is estimated to be about $3 \times 10^{-9}$. If the abundance of gaseous H$_2$O is similar to the value observed in molecular clouds and protostars, $\sim 10^{-7}$, HDO/H$_2$O ratio is 0.01. The fact that the line is a deep absorption line immediately indicates that HDO must be present above the midplane (from where the sub-millimeter continuum is emitted). It must also be present especially in the outer radial regions ($\geq 600$ AU) of the disk since the continuum originates from an extended region. The presence of a large column of HDO in this location was a surprise, since the grain temperatures in this region are below 25 K, and H$_2$O and HDO should be almost entirely frozen out onto grains. Chemical models including thermal desorption of water ice and gas-phase formation of H$_2$O (Aikawa et al. 2002; van Zadelhoff et al. 2003) predict a H$_2$O column of $10^{14}$ cm$^{-2}$ at about 400 AU, only a factor of 5 larger than the observed HDO column. Willacy & Langer (2000) included photo-desorption by a strong stellar UV field and found H$_2$O column densities of about $5 \times 10^{15}$ cm$^{-2}$ at 700 AU. An extended component of HDO (and consequently water) therefore indicates a desorption agent from grain surfaces. Important possibilities are X-rays originating from the star, and penetrating throughout the entire outer disk, and UV photons, either from the star or simply due to the interstellar radiation field.

High energy photons can in principle act to remove H$_2$O molecules from the ice layers on dust grains. X-rays are energetic enough to remove a number of molecules, if sufficient
energy can be concentrated close to the surface of the ice mantle on a grain. This idea has been explored by Najita et al. (2001) who considered X-ray heating of small grains, or spot heating of larger grains. Small grains, or small thermally insulated spots on large grain can be heated strongly enough by a single X-ray absorbed photon to lead to thermal evaporation of part of the ice mantle.

An alternative mechanism is desorption by FUV photons (Willacy & Langer 2000). An FUV photon absorbed in the surface layer of an ice mantle can lead to the release of a molecule into the gas. In this Letter we explore the effect of just the interstellar FUV radiation field irradiating the disk surface of DM Tau. We show that such a scenario leads to a layer of water vapor in the disk surface to an FUV optical depth around unity. The column densities reached in steady state appear to be a viable explanation for the HDO absorption line seen in DM Tau. To show this we developed a simple model of the chemistry leading to the presence of water vapor in irradiated gas containing grains covered by layers of water ice. A much more detailed discussion in the context of a full Photo-Dissociation Region (PDR) model, as well as analytical formulas to estimate H$_2$O column densities under such conditions will be given by Hollenbach et al (2005, in preparation). Here we report the application of this model to the case of DM Tau. A forthcoming paper will present the results of a larger parameter space study, which will explore the dependence of the model predictions especially on the characteristics of the grains (Ceccarelli et al. in preparation).

2. Model description

The model computes the H$_2$O abundance across a protoplanetary disk, as a function of the radius and height. For the physical structure we used the dust density and temperature profile which fits the Spectral Energy Distribution (SED) of DM Tau (Ceccarelli et al. 2005), and shown in Fig. 1. The gas is assumed to be fully coupled with the dust in terms of density distribution and temperature.

Due to the low temperature, the dust grains are covered with an ice layer. In our model, UV photons entering the disk surface are absorbed by dust grains, and cause photo-desorption of water molecules from the ice. Only UV photons absorbed directly at the surface of the ice mantle can desorb a molecule, so that only a small fraction of absorbed photons will cause the ejection of H$_2$O. Laboratory experiments at Lyman $\alpha$ wavelength have shown that the involved yields are typically between $10^{-3}$ and $10^{-2}$ molecules per photon (Westley et al. 1995b). The yield increases to some extent depending on the UV dose in the experiment, apparently because radical formation on the ice surface aids the desorption process (Westley et al. 1995a). It is unclear how important this effect is in astrophysical
environments, and we adopt a conservative value for the yield of $10^{-3}$ molecules per incident FUV ($6 \leq h\nu \leq 13.6$ eV) photon. The yield probably introduce a factor of a few uncertainty into the computations (see below).

The desorption process at a given location will also depend on the attenuated FUV flux, and the rate per unit volume can be written as:

$$k_{\text{des}} = G_0 f_0 Y \exp\left(-\frac{N(H_2)}{N_{\text{uv}}}\right) \sigma_{\text{gr}} n_{\text{gr}},$$

where $G_0$ is the FUV field in Habing (1968) units. $f_0 = 10^8$ photons/cm$^2$/s is the FUV flux for the standard Habing interstellar field ($G_0=1$). $Y$ is the photo-desorption yield. $N_{\text{uv}}$ is H$_2$ column density that gives $\tau_{\text{uv}} = 1$ between 6 and 13.6 eV; we adopted a value equal to $1.8 \times 10^{21}$ cm$^{-2}$ (Tielens & Hollenbach 1985). $\sigma_{\text{gr}}$ is the grain geometrical cross section, equal to $\pi a_{\text{gr}}^2$, where we assumed an average grain size of 0.1 $\mu$m. $n_{\text{gr}}$ is the grain number density. The product $\sigma_{\text{gr}} n_{\text{gr}}$ is approximately $10^{-21}$ cm$^{-2}$ times the gas density $n_{\text{H}_2}$, obtained assuming a gas to dust ratio in mass equal to 1:100. After being released into the gas phase, water either freezes out back onto a grain, or it is photo-dissociated by the FUV photons at the rates:

$$k_{\text{freeze}} = S_{\text{gr}} \sigma_{\text{gr}}^2 n_{\text{gr}} n_{\text{H}_2} < v_{\text{th}} >$$

and

$$k_{\text{phd}} = G_0 I_0 \exp\left(-\frac{N(H_2)}{N_{\text{uv}}}\right) n_{\text{H}_2}$$

where $S_{\text{gr}}$ is the sticking coefficient, for which we use 1 (Burke & Hollenbach 1983). $< v_{\text{th}} >$ is H$_2$O molecule thermal velocity. $I_0 = 5.1 \times 10^{-10}$ s$^{-1}$ (Le Teuff et al. 2000) is the rate of FUV dissociation in unshielded $G_0 = 1$ field.

Gaseous atomic oxygen can freeze out onto grains, where it is assumed to form water ice by reactions with hydrogen atoms on the grain surfaces. O atoms may also form water in the gas phase via the standard sequence of reactions started by the reaction between O and H$_3^+$. The gas phase formation of water thus proceeds at a rate:

$$k_{\text{gas}} = k_{\text{form}} n_O n_{H_3^+}$$

where $k_{\text{form}}$ is equal to $8 \times 10^{-10}$ s$^{-1}$ cm$^{-3}$ (the rate coefficient for the reaction O + H$_3^+ \rightarrow$ OH$^+$ + H$_2$) times 0.33 (the last factor accounts for the fraction of H$_3$O$^+$ recombinations with electrons forming H$_2$O (Le Teuff et al. 2000)). The atomic oxygen abundance is also computed by the steady state equilibrium between formation and destruction processes: photo-dissociation of gas phase water (Eq. (3)) for the formation, and formation of gaseous water via reaction with H$_3^+$ (Eq. (4)) and freezing onto the grains for the destruction of O.
We assume that these reactions are the dominating processes, and that all the oxygen not contained in CO or silicates is contained in O, H$_2$O, and H$_2$O ice.

Finally, the H$_3^+$ abundance is computed as follows. H$_3^+$ is formed by cosmic ray ionization of H$_2$ to form H$_2^+$, followed by the reaction with H$_2$ to form H$_3^+$. In the regions where CO molecules are not frozen onto the grain mantles, H$_3^+$ is destroyed by the reaction with CO. Elsewhere, the H$_3^+$ abundance is computed following the model described in Ceccarelli & Dominik (2005), which takes into account all three deuterated forms of H$_3^+$ and solves the chemical composition by considering the reactions between H$^+$, e$^-$, grains, and H$_3^+$ isotopologues.

3. Discussion

Figure 2 shows the H$_2$O abundance (with respect to H$_2$) across the disk, for a standard interstellar UV field ($G_0 = 1$). Figure 3 shows a vertical cross-section of the chemical species involved in water formation at a radius of 700 AU. Despite the relatively large densities in the disk, water vapor has an abundance of $\sim 3 \times 10^{-7}$ in a large fraction of the outer disk, in the layers just above the midplane, where the A$_V$ to the disk surface is lower than $\sim 5$ mag. By midplane here we mean the region where more than 2/3 of CO molecules are frozen onto the grain mantles. This occurs at an height of about 230 AU at a radius of 700 AU, and 100 AU at a radius of 400 AU. Above this height, CO is desorbed thermally. The gas phase water abundance peaks near the surface where the FUV desorbing flux is high and where the H$_3^+$ abundance is high. In practice, the freeze-out rate of the H$_2$O molecules is larger than the FUV photo-desorption rate of the grain mantles only at densities larger than about $10^7$ cm$^{-3}$. At lower densities, assuming water is in the grain surfaces, water vapor is formed mostly through direct photo-desorption from mantles, and, to a lesser extent, by gas phase reactions occurring among atomic oxygen (a product of H$_2$O photo-dissociation) and H$_3^+$. In the upper layers, atomic oxygen is predicted to be very abundant. The resulting average gas phase H$_2$O column density of a face-on disk is $1.6 \times 10^{15}$ cm$^{-2}$. Figure 4 shows how the column density is distributed as function of the radius. The column density is remarkably constant over most of the disk, although the column does rise slightly with radius.

The first conclusion of our study is that vapor water can indeed be found with relatively high abundances ($\sim 10^{-7} - 10^{-6}$) and column densities ($\sim 1.6 \times 10^{15}$ cm$^{-2}$) in the protoplanetary disk. The gas phase CO abundance has only a minor influence on the gas phase H$_2$O abundance in our model.

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5In our model CO molecules are not photo-desorbed from the mantles, although this is plausible, depending on the structure of the mantles and where on the grain the frozen CO is located. However, the gas phase CO abundance has only a minor influence on the gas phase H$_2$O abundance in our model.
etary disks which surround low luminosity protostars illuminated by the interstellar radiation field (ISRF), like in the case of DM Tau. This is caused by the photo-desorption of the icy grain mantles by the average ISRF. Increasing the FUV field by a factor of ten and hundred leads to H$_2$O column densities larger by only factor 1.5 and 2 respectively. Decreasing the FUV field by a factor ten results in decreasing the H$_2$O column density by a factor a bit more than a factor 2. Therefore, the H$_2$O column density is not sensitive to the addition of a possible FUV field from the central source or a nearby hot star (see Hollenbach et al. 2005 for details and an analytical proof of the insensitivity to G$_o$). The fundamental reason for this insensitivity is that in higher fields, the increased photo-desorption of the ice is balanced by the increased photo-dissociation of gas phase H$_2$O.

As discussed above, the value of the photo-desorption yield, $Y$, is only constrained within a factor roughly three to ten by laboratory experiments. This uncertainty causes an uncertainty in the predicted H$_2$O column density by the same factor. Another important, and poorly known parameter that enters in these computations is the dust-to-gas ratio. In the standard case we assumed the canonical mass dust-to-gas ratio equal to 1%. If this value is increased by a factor ten (which means decreasing by a factor 10 the gas density in the plot of Fig. 1), the H$_2$O column density increases by a factor $\sim 1.2$. On the contrary, a decrease by a factor ten of the dust-to-gas ratio leads to a decrease by a factor 1.2 of the H$_2$O column density. This is due to the fact that the UV optical depth is determined by the dust distribution only and independent of the gas density. As long as photo-desorption, photo-dissociation and freeze-out are the dominant processes, the derived densities and column densities (as opposed to the abundances) of H$_2$O are independent of the gas density. The small changes are due to regions in which the gas formation route of H$_2$O is important. Therefore, also a drastic change in the dust-to-gas ratio does not cause much of a change in the H$_2$O vapor column density. Finally, the results will also depend on the grain size distribution. If much smaller grains than 0.1\,$\mu$m dominate the grain surface area, the balance between the different formation and destruction rates will be shifted. This question will be discussed in a followup paper.

In conclusion, we predict a H$_2$O column density in protostellar disks similar to that surrounding DM Tau of a few times $10^{15}$ cm$^{-2}$, rather insensitive on the external FUV field and/or the dust-to-gas ratio in the disk.

Ceccarelli et al. (2005) reported the detection of HDO in DM Tau, with an observed column density of $\sim 1.6 \times 10^{13}$ cm$^{-2}$. Based on the present theoretical model, the H$_2$O column density is predicted to be $\sim 2 \times 10^{15}$ cm$^{-2}$, within about a factor of a few, given the uncertainties in the yield, FUV field and the dust-to-gas ratio. This implies a HDO/H$_2$O ratio equal to about 1%. This is consistent with estimates of the HDO/H$_2$O ratio in embedded
low mass protostars. Parise et al. (2005) measured a HDO/H$_2$O ratio equal to 3% in the sublimated ices surrounding IRAS16293-2422, and a much lower ($\leq 0.2\%$) value in the outer envelope where the gas phase chemistry dominates the HDO and H$_2$O formation. Note that the large HDO/H$_2$O ratio of 3% refers only to the sublimated ices, which are responsible for the water abundance $3 \times 10^{-6}$ in this object (Ceccarelli et al. 2000). Very likely, the sublimated ices are only the “last coating” of the mantles where the molecular deuteration is the largest, due to the history of ice formation. In agreement with this interpretation, NIR observations of HDO ice have, so far, failed to detect it, at a level of HDO/H$_2$O $\leq 2\%$ (Parise et al. 2003) Therefore, only a small fraction of elemental deuterium is iced on the mantles. The HDO/H$_2$O ratio in DM Tau, equal to $\sim 1\%$, is just slightly lower than the value measured in IRAS16293-2422 and attributed to sublimated ices. If the values were indeed different, this might point to reprocessing of the ices in the disk - however, for this an actual measurement of the vapor water in DM Tau is required. The measurement of the H$_2$O column density would also allow to measure the photo-desorption yield. In addition, measures of the HDO/H$_2$O ratio in protoplanetary disks will probe the history of the ice formation, with important implications for the chemical and isotopic composition of Solar System objects. Based on our model, we predict the ground state transition of H$_2$O at 557 GHz to be in absorption similar to the HDO ground transition at 464 GHz. The line is predicted to be highly optically thick, with $\tau \sim 500$. Unfortunately, neither the currently available ODIN nor the planned HSO satellites will be able to detect the continuum of DM Tau, because of the large beam dilution of the signal from the disk.

4. Conclusions

The results reported in this Letter lead to the following important conclusions:

1. An external UV radiation field as weak as the average Habing field (G$_0=1$) can produce a layer of H$_2$O on top of a protoplanetary disk (like that surrounding DM Tau) with a column of a few times $10^{15}$ cm$^{-2}$.

2. This column density is insensitive to external parameters like the strength of the radiation field: Variations in G$_0$ by two orders of magnitude only change N(H$_2$O) by a factor of 2.

3. Similarly, changing the dust-to-gas ratio (i.e. the gas density at a given dust density) has only weak influence on the derived column densities.

4. Because of the weak dependence on parameters, the measurement of the H$_2$O column density in protoplanetary disks is an excellent tool to measure the photo-desorption yield Y.

5. Combined with previous observations of HDO (Ceccarelli et al. 2005), we predict an HDO/H$_2$O ratio in the outer disk of DM Tau of 0.01, with an uncertainty of about a factor of a few.
6. We predict that the H$_2$O ground state line at 557 GHz is undetectable in DM Tau with ODIN and/or HSO-HIFI observations. Finally, we remark that other molecules trapped in the water ices could also be released into the gas phase, keeping “alive” the gas chemistry in the layers above the midplane of the outer disk.

CD and CC acknowledge Travel support through the Dutch/French van Gogh program, project VGP 78-387 and the hospitality at NASA Ames during the development of this work, during which CD received Travel funds from the University of California, Berkeley. DH acknowledges support from the NASA Astrophysical Theory, Dynamics and Origins of Solar Systems. This work has benefited from research funding from the European Community’s Sixth Framework Programme. We thank the referee Juri Aikawa for a detailed report.
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This preprint was prepared with the AAS LATEX macros v5.2.
Fig. 1.— The logarithm of the gas density (upper panel) and the temperature (lower panel) of the disk surrounding DM Tau, as derived by modeling of the SED (Ceccarelli et al. 2005), and assuming that dust and gas are coupled with $\rho_{\text{dust}}/\rho_{\text{gas}} = 0.01$. 
Fig. 2.— n(H$_2$O)/n(H$_2$) as a function of position in the disk. The solid line shows where the UV optical depth measured vertically to the disk plane is unity: $\tau_{uv} = 1$ (see text). The dashed lines show iso density contours: from the top to the bottom they are $10^4$, $10^5$, $10^6$ and $10^7$ cm$^{-3}$. The white region was excluded from the calculation because of the low density there.
Fig. 3.— The abundances and the visual extinction $A_V$ (from the disk surface) as a function of the height above midplane at 700 AU from the star. The solid and dashed lines show the abundance of H$_2$O and O, respectively. The dashed-dotted and the dotted-dashed lines show the abundance of CO and H$_3^+$. The dotted line indicates the $A_V$. The most important contribution to the H$_2$O column density is produced between $A_V \sim 1$ and $\sim 4$ mag, and a height between 100 and 250 AU. CO freezes out at a height of $\sim 230$ AU. This causes a small increase of the H$_3^+$ abundance, since CO (along with O) is the main destroyer of H$_3^+$. The high abundance of CO at very low $A_V$ may be artificial because we have ignored CO photo-dissociation. The water ice abundance is not shown because it is almost constant $2 \times 10^{-4}$ throughout the plot.
Fig. 4.— Gas-phase H$_2$O column density measured perpendicular to the disk midplane as function of the radius. In the very inner regions the H$_2$O column density decreases because the gas densities at $A_v \sim 1$ are higher, leading to a greater proportion of H$_2$O that is frozen out onto grains as opposed to photo-desorbed. Once the grains are hotter than 100 K ($R \lesssim 30$AU), water will not freeze-out and gas phase abundances will rise again (not shown).