The water ice distribution in Taurus determined by gas–grain chemistry

T. K. Nguyen,1 D. P. Ruffle,2,3 E. Herbst2,4 and D. A. Williams1

1Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT
2Department of Physics, The Ohio State University, Columbus, OH 43210, USA
3School of Chemistry, University of Leeds, Leeds LS2 9JT
4Department of Astronomy, The Ohio State University, Columbus, OH 43210, USA

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ABSTRACT

The detection of water ice in interstellar grain mantles by observation of absorbed radiation from field stars through the Taurus molecular cloud complex has revealed that the column density of water ice increases linearly or nearly linearly with visual extinction except at the lowest values (below AV ∼ 3). Previous explanations of the small or negligible abundance of ice at low extinction have focused on the destruction and desorption of ice by radiation, and have ignored the efficiency of formation of ice. To understand the dependence of the ice column density on AV in more detail and to understand what it tells us about the Taurus dark cloud, we have run gas–grain chemical models under a variety of physical conditions. For higher values of extinction, our models predict that much of the elemental abundance of available oxygen is in the form of ice for evolutionary times greater than about 10^5 yr, and this leads to the observed near-linear relationship between ice column density and AV. For lower extinction, our models show that if any significant amount of ice is still present, its existence can be attributed to great cloud age, to our poor understanding of dust-grain surfaces, or to cloud clumpiness. The first and third explanations pertain only if photodesorption of ice is inefficient.


1 INTRODUCTION

Water ice is the major constituent of grain mantles in dense, cold interstellar clouds (Whittet et al. 1988). As realized by Jones & Williams (1984), ice is synthesized on the surfaces of interstellar grains via the hydrogenation of surface oxygen atoms by hydrogen atoms which land on the grain and diffuse rapidly. The detection of water ice via the use of field stars as sources of infrared radiation, as opposed to internal protostellar sources, has been especially interesting because the cool foreground dust is not contaminated by warm regions surrounding protostellar material. Given the heterogeneity of molecular cloud complexes, a major focus of ice observations has been the determination of the relationship between the ice column density and the visual extinction along various lines of sight through a cloud complex. The two regions studied most closely have been the Taurus and Ophiuchus dark clouds. The former is a rather quiescent region of low mass star formation while the latter is more active because of the presence of nearby hot young stars which enhance the local UV field. Only the Taurus cloud has been studied using background field stars.

Starting with the observations of Harris, Woolf & Rieke (1978) on the ρ Ophiuchus dark cloud and Whittet et al. (1983) on the Taurus cloud, a number of observations have indicated a threshold, or critical, visual extinction, AV, for detection of water ice of ∼3 in Taurus (see e.g. Whittet et al. 1988; Smith, Sellgren & Brooke 1993; Chiar et al. 1995) and ∼12 in Ophiuchus (Tanaka et al. 1990). The most recent paper on Taurus supporting this point of view is that of Whittet et al. (2001), who derive a critical visual extinction of 3.2 ± 0.1. A similar critical extinction has been measured towards the dark cloud R Coronae Australis (Whittet et al. 1996). Two recent studies (Teixeira & Emerson 1999; Murakawa, Tamura & Nagata 2000) show, however, less evidence for individual distinct thresholds in Taurus and ρ Ophiuchus and for much difference between the two cloud complexes. In Taurus, which appears to be the better studied of the two sources, the data of Murakawa et al. (2000), which are solely concerned with field stars as the sources of radiation, show a large scatter in data points at AV ≤ 3, with some lines of sight showing detectable ice features. Although these authors suggest that their data can be interpreted in terms of a variable critical threshold AV of 2–5 for ice detection, it is perhaps simpler to conclude from their data that there is no real threshold at all. Indeed, the data set of Murakawa et al. (2000)
appears to indicate detectable amounts of water ice at extinctions
down to less than unity, but given the significant uncertainty in
their relevant data points (see their fig. 2), as well as difficulties in
determining extinctions, it is unclear whether they have indeed
detected ice at very low extinction.

What all studies seem to agree upon is that above a certain
extinction, there is a clear linear dependence between the ice
column density and $A_V$, at least through an extinction of \( \approx 14 \). At
higher visual extinctions, there may be a break in the ice versus $A_V$
curve if one includes water ice observed towards young stellar
objects (YSOs), as was done by Teixeira & Emerson (1999).

The existence of a critical extinction for the detection of water
ice has been interpreted in terms of photodesorption via external or
internal ultraviolet and infrared photons (Adamson et al. 1988;
Williams, Hartquist & Whittet 1992; Smith et al. 1993) in an
inhomogeneous medium. This interpretation has been maintained
by Murakawa et al. (2000) despite their failure to find a single
threshold extinction for ice in Taurus. Indeed, the lack of a single
critical $A_V$ has been explained in terms of clumpiness.

Although the destruction of ice doubtless plays a role in the ice
versus $A_V$ curve, little attention has been paid to the formation
efficiency of water ice under differing physical conditions. The
need to consider both formation and destruction suggests that a
detailed study of the chemistry of water ice be undertaken under
conditions ranging from low density and low visual extinction to
high density and high visual extinction. It is indeed conceivable
that when ice formation is taken into account, calculated
abundances may show that the ice column density--$A_V$ plot is not
particularly sensitive to the clumpiness of clouds along the lines of
sight.

In this paper, we report the use of chemical models to investigate
water ice abundances over a wide range of physical conditions
relevant to the interstellar medium. Our models incorporate both
gas-phase and diffusive grain surface chemistry. The results we
obtain are used to obtain theoretical plots of ice column density
versus $A_V$ which are then compared with observations for the well
studied Taurus dark cloud. In Section 2 we describe the models
used and in Section 3 we present our results. In Section 4 we
discuss the significance of our findings.

## 2 Model

We use the new gas–grain chemical networks of Ruffle & Herbst
(2000, 2001a, hereafter Papers I and II), in which gas-phase and
grain surface chemistries are linked through accretion and
desorption processes. The networks are based on a diffusive
surface chemistry occurring on an olivine-like material. Developed
in response to simulations of new experimental data on the surface
mobility of hydrogen atoms (Katz et al. 1999), the networks
incorporate slower rates of diffusion of species across grain
surfaces than assumed previously (e.g. Hasegawa, Herbst & Leung
1992; Willacy & Millar 1998). A variety of models have been
developed from the chemical networks. In Paper I, two distinct
models – M1 and M2 – were discussed; these differ in the adopted
surface diffusion rates. In M1, atomic H is the only species with
reduced mobility relative to that used in previous models, and the
diffusion of H is not fully slowed to the extent measured by Katz
et al. (1999). In M2, the atomic hydrogen diffusion rate is indeed
slowed to the measured value, while the diffusion rates of all other
species are slowed proportionally. In both models, desorption of
surface species occurs via thermal evaporation (which returns only
the most weakly bound species to the gas phase at low grain

In Paper II, M1 and M2 were extended to incorporate surface
photochemistry and renamed P1 and P2, respectively. Terms were
included for both the external background radiation field and the
cosmic ray induced field. The surface photochemistry takes the
form of photodissociation, with products remaining on the surface.
Differences with the calculated gas-phase and surface abundances
of the earlier M1 and M2 models occur only at very long times for
dense quiescent sources in molecular clouds. In yet another paper,
the models (as well as analogous ones incorporating diffusion on
amorphous carbon) were used to study the abundance of carbon
dioxide ice (Ruffle & Herbst 2001b).

Here we introduce new models to incorporate photodesorption
following photodissociation of water ice, which requires a
threshold wavelength of \( \approx 200 \text{ nm} \). The cross-sections for
photodissociation are such that its efficiency per sufficiently
energetic photon is approximately 0.01 per monolayer if the
monolayer is pure ice. Although photodesorption via visible
photons appears to be very inefficient (Bourdon, Prince, & Duley
1982), there is some evidence for photodesorption following
photodissociation of water ice with UV photons. In particular,
Westley et al. (1995) found that pure cold ice can undergo
photodesorption at the Lyman \( \alpha \) wavelength (122 nm) at
efficiencies up to 0.01. Although the efficiency apparently refers
to the total of all monolayers of ice up to the penetration depth of
450 \( \text{ A} \text{˚} \), Westley et al. (1995) assume that most desorption takes
place in the outer monolayer. In addition, this efficiency is reached
only after the ice is bombarded by a large number of photons. If, as
suggested by the authors, the process involves intermediate
formation of surface OH radicals via photodissociation of water
followed by photodesorption of the radicals or their reaction with
excited water molecules, then it is likely to be even less efficient in
the interstellar medium, where H atoms from the gas can
recombine with surface OH radicals prior to their desorption.

In Paper II, models with limited photodesorption were discussed
for the case where all hydrogen atoms produced via surface
photochemistry are ejected into the gas phase. The results of these
models for cold quiescent sources were found to be identical to
those in which the atomic H is retained on the surface because H
atoms are sufficiently abundant in dense cores that enough atomic
H arrives on the surface to replace atoms ejected. In this paper, we
explore the effect of allowing both H atoms and OH radicals
produced via photodissociation of surface water molecules to
desorb. We assume as an extreme case that the ejection of H and
OH is 100 per cent efficient following photodissociation, which
implies an overall efficiency per energetic photon per monolayer of
0.01. Since we allow the process to occur for up to 100 monolayers
of ice, our efficiency is far higher than the maximum efficiency
determined by Westley et al. (1995) with Lyman \( \alpha \) photons except
when only one monolayer of ice is present. The versions of the
models P1 and P2 which incorporate this photodesorption
mechanism are labelled Z1 and Z2. In Table 1 the four models
used in this paper, P1, P2, Z1 and Z2, are compared.

In the models, grains with radii of 0.1 \( \mu \text{m} \) and \( 10^6 \) \( ^{2} \) binding sites
are assumed. We adopt a value of the sticking coefficient of 0.5.
The standard value for the cosmic ray ionization rate $\zeta$ of \( 1.3 \times 10^{-17} \text{ s}^{-1} \) is used. As in Papers I and II, we use the ‘low metal’
values for the initial elemental abundances, following Lee, Betbens
depending on the density. We note that the use of molecular rather than atomic hydrogen has been employed as the initial form of the element. The kinetic equations used for surface diffusion are taken from the modified rate equation approach of Caselli, Hasegawa & Herbst (1998), Shalabiea, Caselli & Herbst (1998) and Stantcheva, Caselli & Herbst (1996), which can be found in Papers I and II.

The notation \( a(b) \) implies \( a \times 10^b \). Based originally on diffuse cloud data (Bohlin, Savage & Drake 1978) but consistent with other sources. We ignore all lesser contributions to the ice column density along the line of sight. The column density of water ice, \( N(\text{H}_2\text{O} \text{ ice}) \), is calculated from the relation

\[
N(\text{H}_2\text{O} \text{ ice}) = x(\text{H}_2\text{O} \text{ ice}) \times n_H \times L,
\]

where \( x \) denotes the fractional abundance of solid water determined in our model calculations. Substituting in the result of equation (1) yields

\[
N(\text{H}_2\text{O} \text{ ice}) = x(\text{H}_2\text{O} \text{ ice}) \times 1.6 \times 10^{21} \times A_V.
\]

Thus, if \( x \) is constant, a plot of the column density of ice versus the visual extinction should be a straight line with slope \( x \times 1.6 \times 10^{21} \).

In addition to studying the dependence of the water ice abundance on \( A_V \), we also consider the dependence of condensed phase CO on \( A_V \) since this has been studied observationally for the Taurus dark cloud, although to nowhere near the extent of the water ice studies.

### 3 RESULTS

#### 3.1 Water ice versus extinction

The calculated column density of water ice versus \( A_V \), over the range \( 0.5 \leq A_V \leq 20 \) at assorted times is plotted for models P1 and Z1 in Fig. 1 and for models P2 and Z2 in Fig. 2. For P1 and P2, values are shown for \( 10^5 \text{ yr} \) (––), \( 10^6 \text{ yr} \) (— –) and \( 10^7 \text{ yr} \) (– – –), whereas for Z1 and Z2, results are given at only \( 10^6 \text{ yr} \) (– –) and \( 10^7 \text{ yr} \) (– – –) since the results at \( 10^5 \text{ yr} \) do not differ from those of P1 and P2. In addition to the calculated results, the observational results for the Taurus dark cloud of Murakawa et al. (2000; denoted by diamonds), Whittet et al. (2001; denoted by stars) and of Teixeira & Emerson (1999; denoted by squares) are included in the figures. Uncertainties for selected data points of Murakawa et al. are shown. Data at higher visual extinction are not included. Finally, the solid line in each figure represents the column density obtained if water ice is assumed to have a constant fractional abundance of

\[
L(\text{cm}) = 1.6 \times 10^{21} \times A_V/n_H,
\]

Table 1. Comparison of models with olivine-like grain surfaces.

<table>
<thead>
<tr>
<th>Model</th>
<th>H diffusion</th>
<th>Diffusion of other species</th>
<th>OH photodesorption</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>slow</td>
<td>unaltered</td>
<td>no</td>
</tr>
<tr>
<td>P2</td>
<td>very slow</td>
<td>very slow</td>
<td>no</td>
</tr>
<tr>
<td>Z1</td>
<td>slow</td>
<td>unaltered</td>
<td>yes</td>
</tr>
<tr>
<td>Z2</td>
<td>very slow</td>
<td>very slow</td>
<td>yes</td>
</tr>
</tbody>
</table>

*All species other than H and H\(_2\). Details concerning the diffusion rates can be found in Papers I and II.

Table 2. Initial elemental fractional abundances.

<table>
<thead>
<tr>
<th>Element (initial form)</th>
<th>Fractional abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.00</td>
</tr>
<tr>
<td>He</td>
<td>1.4(–1)</td>
</tr>
<tr>
<td>N</td>
<td>2.14(–5)</td>
</tr>
<tr>
<td>O</td>
<td>1.76(–4)</td>
</tr>
<tr>
<td>C(^+)</td>
<td>7.3(–5)</td>
</tr>
<tr>
<td>S(^+)</td>
<td>8.0(–8)</td>
</tr>
<tr>
<td>Si(^+)</td>
<td>8.0(–9)</td>
</tr>
<tr>
<td>Fe(^+)</td>
<td>3.0(–9)</td>
</tr>
<tr>
<td>Na(^+)</td>
<td>2.0(–9)</td>
</tr>
<tr>
<td>Mg(^+)</td>
<td>7.0(–9)</td>
</tr>
<tr>
<td>P(^+)</td>
<td>3.0(–9)</td>
</tr>
<tr>
<td>Cl(^+)</td>
<td>4.0(–9)</td>
</tr>
</tbody>
</table>

Table 3. Comparison of selected model conditions.

<table>
<thead>
<tr>
<th>( A_V ) (mag)</th>
<th>( n_H ) (cm(^{-3}))</th>
<th>( T ) (K)</th>
<th>( L ) (cm)</th>
<th>Initial form of hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>1.0(02)</td>
<td>25</td>
<td>8.0(18)</td>
<td>Atomic</td>
</tr>
<tr>
<td>1</td>
<td>5.0(02)</td>
<td>20</td>
<td>3.2(18)</td>
<td>Atomic</td>
</tr>
<tr>
<td>3</td>
<td>1.0(03)</td>
<td>15</td>
<td>4.8(18)</td>
<td>Atomic</td>
</tr>
<tr>
<td>5</td>
<td>5.0(03)</td>
<td>10</td>
<td>1.0(18)</td>
<td>Atomic</td>
</tr>
<tr>
<td>10</td>
<td>2.0(04)</td>
<td>10</td>
<td>8.0(17)</td>
<td>Molecular</td>
</tr>
<tr>
<td>15</td>
<td>5.0(04)</td>
<td>10</td>
<td>4.8(17)</td>
<td>Molecular</td>
</tr>
<tr>
<td>20</td>
<td>1.0(05)</td>
<td>10</td>
<td>3.2(17)</td>
<td>Molecular</td>
</tr>
</tbody>
</table>

The notation \( a(b) \) implies \( a \times 10^b \).
$1.8 \times 10^{-4}$ cm$^{-3}$, the maximum allowable given the abundance of oxygen used, at all values of $A_V$.

Postponing a detailed discussion of the results at low $A_V$ ($0.5 \leq A_V \leq 6$) until later, we see from the figures that the calculated results at higher $A_V$ show (a) a linear to near-linear relationship between the water column density and $A_V$ for all models and times used, with a slope similar to the observed data, and (b) an increasing water abundance with increasing time, especially for models P1 and P2, in which there is no photodesorption. Moreover, the observational data are reasonably bracketed by the results of all models at $10^5$ yr, which lie slightly below almost all of the observational points, and all models at $10^6$ yr, which lie either slightly above them (P1 and P2) or above most of them (Z1 and Z2). These data are consistent with a constant fractional abundance of water ice equal to $\approx 30–40$ per cent of the oxygen elemental abundance once $A_V$ exceeds 5. Some data at higher visual extinction than shown indicate even higher ice abundances (Teixeira & Emerson 1999). Since the ordinate is linear, all model results at all times lie within a factor of 2–3 of virtually all the observed ice column densities for $A_V > 5$.

If there is evidence for clumpiness along the line of sight, it is likely to occur at low $A_V$ since small high density clumps with large fractional abundances of water ice will strongly affect the results. In Fig. 3, we expand the low $A_V$ results given in Figs 1 and 2.

Figure 1. Calculated and observed column densities of water ice as a function of $A_V$ over the range $0 \leq A_V \leq 20$ for Taurus. Results for model P1 are given at three times: $\cdots$ denotes $10^5$ yr, $\cdots$ depicts $10^6$ yr and $\times \times$ represents $10^7$ yr. Results for model Z1 are given at two times: $\cdots \cdots$ depicts $10^6$ yr whilst $\cdots \cdots$ denotes $10^7$ yr. Diamonds represent the observations of Murakawa et al. (2000), stars represent those of Whittet et al. (2001) and squares those of Teixeira & Emerson (1999).

Figure 2. Calculated and observed column densities of water ice as a function of $A_V$ over the range $0 \leq A_V \leq 20$ for Taurus. Results for model P2 are given at three times: $\cdots \cdots$ denotes $10^5$ yr, $\cdots \cdots$ depicts $10^6$ yr and $\times \times$ represents $10^7$ yr. Results for model Z2 are given at two times: $\cdots \cdots$ depicts $10^6$ yr whilst $\cdots \cdots$ denotes $10^7$ yr. Diamonds represent the observations of Murakawa et al. (2000), stars represent those of Whittet et al. (2001) and squares those of Teixeira & Emerson (1999).
The water ice distribution in Taurus

The data of Murakawa et al. (2000) indicate that there may be lines of sight with $AV$ as low as 0.5 which show a significant column density ($<10^{17}$ cm$^{-2}$) of water ice. At these low $AV$, the data of Teixeira & Emerson (1999) represent upper limits only. A variety of model results are shown in Fig. 3. Since the four models produce similar results at $10^5$ yr, results for only one model (P1) are plotted at this time. Values are displayed for P1 at $10^5$ yr (---), $10^6$ yr (—) and $10^7$ yr (–). Results for Z2 have not been included in Fig. 3 as they are very similar to those for Z1.

It is useful for the purpose of comparison between theory and observation to divide the low $AV$ range into two sub-ranges: 0.5–3 and 3–6. Whether or not water ice has been detected in the former range is controversial (Whittet et al. 2001), while the latter range is above the standard extinction threshold. The $AV$ = 0.5–3 range is fit well by our models, which can be considered to represent translucent sources, as long as the time significantly exceeds $10^5$ yr, a rather short dynamical time for all but dense clouds. Most of the column densities lie between results for models Z1/Z2 at $10^6–7$ yr and models P1/P2 at $10^6$ yr. The former models, which include a mechanism for photodesorption of water ice, contain results which lie somewhat below the data points, while the latter models contain results which are somewhat above the data. Fine-tuning the time for P1/P2 or reducing the efficiency of photodesorption for Z1/Z2 could improve the agreement even more.

The $AV$ = 0.5–3 range is represented by diffuse to weakly translucent cloud models. These clouds are likely to be dynamically old, and so it is reasonable to consider results at a time in the vicinity of $10^7$ yr. At this time, there is a strong difference between our P1 and P2 model results, on the one hand, and our Z1 and Z2 model results on the other hand. The P1 model results lie near or somewhat below much of the Murakawa et al. (2000) data while the P2 model results lie somewhat above most of the data. A somewhat reduced time for P2 and a somewhat longer time for P1 would reproduce the data better. The Z1 and Z2 models predict very low abundances, because of the photodesorption mechanism, which is very important for low extinction sources. Thus, the Z1 and Z2 model results are incompatible with the Murakawa et al. data but strongly support the existence of a critical extinction of $<3$ (see Fig. 3).

Towards the low end of the 0.5–3 extinction range, we cannot reproduce the non-zero Murakawa et al. data with any of our single point calculations! We simply cannot produce significant amounts of water ice for $AV = 0.5$, while for $AV = 1$, most of our models

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**Table 4.** Column density (cm$^{-2}$) of H$_2$O ice for model P2 with $AV = 1, 3, 5$ and $10$ for sticking coefficients, $S$, of 0.5 and 1.

<table>
<thead>
<tr>
<th>Time (yr)</th>
<th>$AV = 1$</th>
<th>$AV = 3$</th>
<th>$AV = 5$</th>
<th>$AV = 10$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S = 0.5$</td>
<td>1.5(13)</td>
<td>6.2(13)</td>
<td>7.7(14)</td>
<td>5.3(15)</td>
</tr>
<tr>
<td>$S = 1.0$</td>
<td>1.5(14)</td>
<td>6.2(13)</td>
<td>7.7(14)</td>
<td>5.3(15)</td>
</tr>
<tr>
<td>$S = 0.5$</td>
<td>1.4(15)</td>
<td>6.1(15)</td>
<td>7.7(15)</td>
<td>5.3(16)</td>
</tr>
<tr>
<td>$S = 1.0$</td>
<td>1.5(15)</td>
<td>6.2(15)</td>
<td>7.7(15)</td>
<td>5.3(16)</td>
</tr>
<tr>
<td>$S = 0.5$</td>
<td>1.5(16)</td>
<td>6.3(16)</td>
<td>7.8(16)</td>
<td>5.4(17)</td>
</tr>
<tr>
<td>$S = 1.0$</td>
<td>1.5(16)</td>
<td>6.3(16)</td>
<td>7.8(16)</td>
<td>5.4(17)</td>
</tr>
</tbody>
</table>

The notation $a(b)$ implies $a \times 10^b$. 

---

Figure 3. Calculated and observed column densities of water ice as a function of $AV$ over the limited range $0 \leq AV \leq 6$ for Taurus. For model P1, --- depicts $10^5$ yr and -- represents $10^6$ yr. For P2, --- depicts $10^6$ yr whilst --- denotes $10^7$ yr. For Z1, $10^6$ yr is represented by -- and -- represents $10^7$ yr. The observed values are once more represented by diamonds (Murakawa et al. 2000), stars (Whittet et al. 2001) and squares (Teixeira & Emerson 1999).
predict very low abundances of water at times through \(10^7\) yr. The lines of sight with supposedly large ice column densities of almost \(10^{17}\) cm\(^{-2}\) imply fractional ice abundances near \(5 \times 10^{-5}\). This value exceeds that of our most prolific model (P2) for ice production at \(A_V = 1\) by a factor of 5 or so at a time of \(10^7\) yr. If the non-zero ice points at very low extinction are real, it is tempting to conclude that small clumps of high density are the cause although there are other explanations. For example, in models without photodesorption, the water-ice abundances build up as the clouds age; at a time of \(10^5\) yr, for example, P2 yields a very large column density of \(1.3 \times 10^{17}\) cm\(^{-2}\) at \(A_V = 1\). The formation of water ice, although inefficient, is inexorable in models without photodesorption, as long as \(A_V\) is not less than unity. The age needed for development of a significant amount of ice can be reduced considerably if we increase the sticking coefficient \(S\) for gas-phase species striking grains from 0.5 to unity. In Table 4, calculated column densities for ice using model P2 are tabulated for times through \(10^5\) yr and \(A_V = 1, 3, 5, 10\) for \(S = 0.5\) and 1. In particular, at a time of \(10^5\) yr, use of \(S = 1\) in model P2 leads to a column density of \(6.6 \times 10^{16}\) cm\(^{-2}\) at \(A_V = 1\), in good agreement with the high-ice, low extinction Murakawa et al. (2000) data. Other explanations for the possibly non-zero ice points at very low extinction are given in Section 4.

### 3.2 Condensed phase CO versus extinction

Teixeira & Emerson (1999) have studied the dependence of the condensed phase CO column density on \(A_V\) in Taurus. Their data (represented by squares, and of necessity including YSOs) are compared with our results for models P1 and Z1 in Fig. 4. The results for models P2 and Z2 are not significantly different. It can be seen that CO ice appears to become detectable at \(A_V = 3\), and that its column density gradually increases with increasing \(A_V\), albeit with much scatter. Our model results generally agree with the observational data. In Fig. 4, we use the same symbols for model and time as in Fig. 1. Since the models produce similar results at \(10^5\) yr, once again only one model is plotted at this time. The \(10^6\) yr line for model Z1 has also been removed as it is very similar to model P1.

Unlike ice, condensed phase CO cannot be a chronometer for any models, since its abundance does not build up on grains inexorably. It is produced in the gas phase and condenses onto grain mantles, where it can react slowly to produce species such as formaldehyde and methanol.

### 4 Discussion

With our current gas–grain chemical models (Table 1; Papers I and II), we have attempted to simulate the relationship between the water ice column density and visual extinction seen in the direction of the Taurus dark cloud. According to the most recent observations (Teixeira & Emerson 1999; Murakawa et al. 2000; Whittet et al. 2001), there is a linear relationship between the two quantities which extends down from \(A_V = 20\) to rather low extinction, at which point there may be a critical extinction of \(A_V \approx 3\), below which there is no water ice (Whittet et al. 2001), or there may be lines of sight with little extinction which do show a considerable amount of ice (Murakawa et al. 2000).

Assorted models were run for sources with different but fixed conditions, ranging from diffuse to dense, and characterized by assumed values of gas densities, temperatures and \(A_V\). The model results are concentrations of gas-phase and condensed-phase species as a function of time, from which column densities can be estimated. The ice column density along any line of sight in Taurus was assumed to be determined by one dominant type of source, as listed in Table 3, which means that the possibility of several important clumps along a line of sight was not taken into account.

The model results can explain most and possibly all of the observed relationship between ice column density and \(A_V\) without additional assumptions. For the higher values of visual extinction (\(A_V \geq 6\)), the models predict that much of the elemental abundance of oxygen is in the form of water ice at times after \(10^7\) yr. This leads to linear or near-linear relationships between ice column density and \(A_V\). For the models without photodesorption of water, the ice abundance builds up with time, while for those presented in this paper.
models with photodesorption, the build-up is much less dramatic. There is no single time of perfect agreement over the whole range of $A_V$, which is expected since the denser objects doubtless have shorter dynamical lifetimes. For $A_V \approx 6$, the data are fit best by assorted models at times between $10^7$ and $10^9$ yr, while for somewhat lower $A_V$ in the range 3–6, the data are fit well by models with longer lifetimes, depending specifically on whether photodesorption is included.

For the range $A_V = 0.5–3$, observational data differ as to whether or not water ice can be detected. Within the constraints of our olivine-based models and single source conditions along any given line of sight, the major variable, which can lead to the production of water ice under conditions of low extinction, is the lifetime of the source since water ice builds up inexorably in models (P1 and P2) without photodesorption. Simply put, objects with high ice abundance and low extinction have remained cold for very long periods of time. The actual ages needed are sensitive to the sticking efficiency employed. This explanation is only useful for models without photodesorption. Models with efficient photodesorption, on the other hand, show little water ice development at any time in this range of extinction, and are thus in agreement with a critical value for extinction (Whittet et al. 2001).

A second explanation for the possibility of ice at low extinction is the diversity of grain surfaces, because the formation of water ice can have different rates on surfaces other than olivine. Ruffle & Herbst (2001b) have recently developed a model which includes diffusive chemistry on amorphous carbon. On this surface, adsorbs bind more strongly than on olivine, and evaporation is less efficient at diffuse cloud temperatures. Consequently, the formation of water is also more efficient. For example, model results show an appreciable build up of water ice for $A_V = 1$ by $3 \times 10^6$ yr. As another example, current calculations show that surface ice on graphite may occur up to much higher temperatures than on amorphous carbon via a non-diffusive mechanism known as the Eley–Rideal process (Meijer et al. 2001). It must also be remembered that once a monolayer of ice is formed (corresponding to a column density of $1.6 \times 10^{15}$ cm$^{-2}$ at $A_V = 1$), the characteristics of the original surface will change appreciably and begin to resemble those of amorphous ice. Although a recent experimental study of H atom diffusion on amorphous ice shows that molecular hydrogen can be formed on such a surface at low temperature (Manicò et al. 2001), detailed parameters for the motion, which would allow us to model surface chemistry on ice, were not determined. From theoretical work on H diffusion on amorphous ice (Takahashi 2000), it appears that the parameters for diffusive motion (desorption energy, barrier against diffusion), although likely to have a range of values on this complex surface, more closely resemble those used in our model for amorphous carbon than those used for olivine. Thus, if a monolayer of ice can be formed under the harsh conditions of diffuse clouds on a surface such as amorphous carbon, the initial monolayer may ‘catalyse’ the subsequent formation of further monolayers.

A third explanation, discussed in some detail by Murakawa et al. (2000), is that any ice at low $A_V$ is caused by clumpiness along the line of sight, which is to be expected given the degree of inhomogeneity perpendicular to this direction. To fully explore this explanation requires a much more complex series of model calculations than presented here, with a detailed treatment of radiative transfer. Nevertheless, one can use the following argument to gauge this possibility. In our current calculations, an extinction of 1 is interpreted in terms of a diffuse cloud. Alternative interpretations (taken from Table 3) could be (a) two clumps at density $5 \times 10^3$ cm$^{-3}$ and length $1.6 \times 10^7$ cm or one clump at density $2 \times 10^6$ cm$^{-3}$ and length $8.0 \times 10^6$ cm. For model P2, we obtain a total ice column density of $3 \times 10^{15}$ cm$^{-2}$ for both alternative scenarios at $10^7$ yr, far in excess of the value of $1.6 \times 10^{16}$ cm$^{-2}$ obtained for the diffuse cloud case. It is perhaps more reasonable to consider smaller ages for the clumps. If we consider an age of $3 \times 10^5$ yr, the enhancement is more modest but still noticeable, with total computed ice column densities of $3 \times 10^{16}$ cm$^{-2}$ for the two-clump case and $8 \times 10^{15}$ cm$^{-2}$ for the one-clump case. For the model Z2, which contains ice photodesorption via photodissociation, the clump enhancement is greater although the initial diffuse cloud value is much smaller. At an age of $1 \times 10^7$ yr, the computed $A_V = 1$ ice column density in the diffuse cloud case is a very low $1 \times 10^{16}$ cm$^{-2}$; while the column densities for the two-clump and one-clump cases are $5 \times 10^{15}$ cm$^{-2}$ and $2 \times 10^{14}$ cm$^{-2}$, respectively, at all times after $10^7$ yr. These enhanced values are still well below the high-ice data points of Murakawa et al. (2000) at very low extinction. It appears then that altered model results incorporating cloud clumpiness are consistent or inconsistent with the high ice, low extinction data points of Murakawa et al. depending upon whether or not photodesorption of ice is not or is efficient.

In summary, if photodesorption of water via photodissociation is inefficient under interstellar conditions, we can possibly account for relatively large abundances of water ice at $A_V \lesssim 3$ by great age, possibly by surface chemistry on initial surfaces other than olivine, followed by formation on ice itself, and by small dense clumps of material along the line of sight. If, on the other hand, photodesorption of ice is efficient, the first and third explanations do not appear to help sufficiently, leaving only the second as a possibility. Absent this possibility, our results from the Z1 and Z2 models are in close accord with the view that below a critical extinction of $\approx 3$ no ice exists. These models with efficient photodesorption are partially supported by the photodesorption studies of Westley et al. (1995) when not too many monolayers of ice are present. It is clear though that a full understanding of the proper low-extinction ice versus $A_V$ relation in Taurus and other sources will require increases in our understanding of surface chemistry, especially on amorphous ice, and of photodesorption on a variety of surfaces.

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