On the encounter desorption of hydrogen atoms on an ice mantle

Qiang Chang¹, Xu-Li Zheng², Xia Zhang², Dong-Hui Quan²,³, Yang Lu⁴, Qing-Kuan Meng¹, Xiao-Hu Li² and Long-Fei Chen²

¹ School of Physics and Optoeletronic Engineering, Shandong University of Technology, Zibo 255000, China; changqiang@sdtu.edu.cn
² Xinjiang Astronomical Observatory, Chinese Academy of Sciences, Urumqi 830011, China; zhangx@xao.ac.cn
³ Department of Chemistry, Eastern Kentucky University, Richmond, KY 40475, USA
⁴ School of Physics & Astronomy, Sun Yat-Sen University, Zhuhai 519082, China

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Abstract At low temperatures (∼10 K), hydrogen atoms can diffuse quickly on grain ice mantles and frequently encounter hydrogen molecules, which cover a notable fraction of grain surface. The desorption energy of H atoms on H₂ substrates is much less than that on water ice. The H atom encounter desorption mechanism is adopted to study the enhanced desorption of H atoms on H₂ substrates. Using a small reaction network, we show that the steady-state surface H abundances predicted by the rate equation model that includes H atom encounter desorption agree reasonably well with the results from the more rigorous microscopic Monte Carlo method. For a full gas-grain model, H atom encounter desorption can reduce surface H abundances. Therefore, if a model adopts the encounter desorption of H atoms, it becomes more difficult for hydrogenation products such as methanol to form, but it is easier for C, O and N atoms to bond with each other on grain surfaces.

Key words: astrochemistry — ISM: abundances — ISM: molecules

1 INTRODUCTION

The grain ice mantle is observed to be mainly composed of water ice (Oberg et al. 2011), thus, the substrate for the grain-surface chemical reactions is usually assumed to be water ice only in the traditional astrochemical models (Hasegawa et al. 1992; Hasegawa & Herbst 1993; Garrod & Herbst 2006). However, this assumption may not be valid if the grain ice mantle is composed of other surface species on which the desorption energies of surface species differ significantly from these on water ice. For instance, the desorption energy of surface species on the H₂ substrate is more than one order of magnitude lower than that on water ice (Cuppen & Herbst 2007). If we still assume the substrates are water ice only, hydrogen molecules may be depleted in the gas phase and are frozen on grains at low temperatures and high densities (Hincelin et al. 2015). However, to the best of our knowledge, the depletion of H₂ has never been reported. So, for better astrochemical modeling, there should be at least two kinds of substrates on grain surface, water and molecular hydrogen in a chemical model.

In order to consider the much lower desorption energy of surface species on molecular hydrogen in astrochemical models, Morata & Hasegawa (2013) made a crude approximation and assumed that the dust grains are completely covered by H₂ at 10 K. However, to the best of our knowledge, the validity of this assumption has not been proved. Garrod & Pauly (2011) suggested another approach to solve the problem. They used the fractional coverage of surface H₂ to adjust the desorption energies on water ice in their models. The adjusted desorption energies are named the effective binding energies. One major limitation of this approach is that an empirical modifying factor has to be used to calculate the effective binding energies.

It is straightforward to include both H₂ and water ice substrates in the microscopic Monte Carlo (MC) models (Chang et al. 2005; Cuppen et al. 2017). This numerical approach keeps track of the trajectory of each surface species when it hops among binding sites. If a
surface species hops into a site where there is one H₂ molecule, the substrate for that the surface species is H₂ ice. Otherwise, the substrate is water ice. However, this numerical approach is computationally expensive when the surface temperatures are high (≥15 K) because the hopping events of surface species consume most CPU time at high temperatures. Therefore, so far this approach can only be used to simulate the chemistry of cold sources such as the dark molecular clouds.

Recently, a new mechanism called the encounter desorption was suggested so that surface H₂ abundances on heterogeneous grain surface can be calculated by the rate equation (RE) approach (Hincelin et al. 2015). This mechanism considers the desorption of hydrogen molecules when they encounter other surface H₂ molecules. The implementation of this mechanism in astrochemical models is very convenient. Only one extra surface reaction gH₂ + gH₂ → H₂ + gH₂ has to be added into the chemical reaction network, where the letter g designates surface species. Moreover, the rate coefficient of the extra surface reaction has a simple analytical formula (Hincelin et al. 2015). The calculated surface H₂ abundances by the RE approach from models including this reaction agree reasonably well with the results calculated by the microscopic MC method.

Hydrogen atoms can diffuse almost as fast as gH₂ on the grain surface, so they should encounter H₂ frequently on grain surfaces if H₂ is abundant. The desorption energy of H atoms on gH₂ substrates is about 45 K (Cuppen & Herbst 2007), so H atoms should sublime quickly when they encounter gH₂ molecules just like molecular hydrogen. Because the surface chemistry is dominated by hydrogenation reactions when the grain temperature is around 10 K, grain surface chemistry is likely to be affected if the encounter desorption of H atoms is included in models.

In this work, we investigate how grain surface chemistry is affected by the encounter desorption of H atoms. The paper is organized as follows. In Section 2, we derive a math formula for the rate coefficient of H atom encounter desorption on grain surface. In Section 3, we show that for a simple reaction network that include the encounter desorption of H atoms, the surface H abundances calculated by the RE approach agree reasonably well with those predicted by the microscopic MC approach. In Section 4, we simulate a full gas-grain reaction network that includes the encounter desorption of gH₂ molecules and gH atoms and present the impacts of gH atoms encounter desorption on the surface chemistry in cold cores. In Section 5, we summarize our findings and draw the conclusions.

2 THE ENCOUNTER DESORPTION OF H SURFACE ATOMS

Following the gH₂ encounter desorption mechanism, in order to include the gH encounter desorption mechanism in a chemical model, we can simply add an extra reaction, gH + gH₂ → H + gH₂, to the chemical reaction network. Before deriving the rate coefficient for this reaction, we first review the encounter desorption mechanism of gH₂ and derive the rate coefficient for the reaction gH₂ + gH₂ → H₂ + gH₂.

Figure 1 shows the diffusion of gH₂ on a heterogeneous ice mantle composed of water ice and H₂. We assume that the ice mantle is mainly composed of water ice, which agrees with observations toward cold sources (Oberg et al. 2011). When a hydrogen molecule hops from a water ice binding site to another site that is occupied by gH₂ as shown in the figure, gH₂ desorption competes with the hopping events of gH₂. The probability that gH₂ desorbs is given by the following equation (Chang et al. 2005),

\[ P_{H_2} = \frac{b_{H_2}H_2}{b_{H_2}H_2 + k_{H_2}H_2} \]  

where \( b_{H_2}H_2 \) and \( k_{H_2}H_2 \) are the thermal desorption and hopping rates of gH₂ on gH₂ substrates respectively. The thermal desorption rate of gH₂ on gH₂ substrates is \( b_{H_2}H_2 = \nu \exp(-E_{D_{H_2}H_2}/T) \) while the hopping rate of gH₂ on gH₂ substrates is \( k_{H_2}H_2 = \nu \exp(-E_{b_{H_2}H_2}/T) \), where \( E_{D_{H_2}H_2} \) and \( E_{b_{H_2}H_2} \) are desorption energy and diffusion barrier of gH₂ on gH₂ substrates. Assuming the number of binding sites occupied by gH₂ is much smaller than the total number of binding sites on the grain surface, the rate coefficient for two hydrogen molecules to encounter is given by

\[ r_{H_2H_2} = \frac{2k_{H_2}H_2O}{S} \]  

where \( k_{H_2}H_2O \) is the hopping rate of gH₂ on water ice while \( S \) is the total number of binding sites on the grain surface. Similarly, \( k_{H_2}H_2O = \nu \exp(-E_{b_{H_2}H_2O}/T) \), where \( E_{b_{H_2}H_2O} \) is the diffusion barrier of gH₂ on water ice. Finally, we have the rate coefficient for the reaction gH₂ + gH₂ → H₂ + gH₂, which has a simple analytical form,

\[ r_{enc_{H_2}} = r_{H_2H_2}P_{H_2} \]  

Figure 1 also shows the diffusion of gh on the grain ice mantle and the encounter of gH and gH₂. The rate coefficient for the reaction gH + gH₂ → H + gH₂, \( r_{enc_{H_2}} \)
can be derived as follows. First, the probability that a gH atom desorbs into the gas phase after it encounters a gH₂ molecule is

$$ P_{\text{HH}_2} = \frac{b_{\text{HH}_2}}{b_{\text{HH}_2} + k_{\text{HH}_2}}, \quad (4) $$

where $b_{\text{HH}_2} = \nu \exp(-E_{\text{DHH}_2}/T)$ and $k_{\text{HH}_2} = \nu \exp(-E_{\text{bHH}_2}/T)$ are the thermal desorption and hopping rates of gH on gH₂ substrates respectively. The two parameters $E_{\text{DHH}_2}$ and $E_{\text{bHH}_2}$ are the desorption energy and diffusion barrier of gH on gH₂ respectively. The gH and gH₂ encounter rate coefficient is

$$ r_{\text{HH}_2} = \frac{k_{\text{HH}_2 \text{O}} + k_{\text{HH}_2 \text{O}}}{S}, \quad (5) $$

where $k_{\text{HH}_2 \text{O}}$ is the hopping rate of gH on water ice, which is dependent on the diffusion barrier of gH on water ice, $k_{\text{HH}_2 \text{O}} = \nu \exp(-E_{\text{bHH}_2}/T)$. There are two possible scenarios where hydrogen atoms encounter hydrogen molecules. Either a gH atom hops into a site already occupied by gH₂ or vice versa. The encounter desorption of gH only occurs in the first case. We will explain the reason in the next section, where the microscopic MC method will be briefly introduced. The probability for the first case to occur is $P = \frac{k_{\text{HH}_2 \text{O}}}{k_{\text{HH}_2 \text{O}} + k_{\text{HH}_2 \text{O}}}$ Finally we have

$$ r_{\text{encHH}_2} = \frac{r_{\text{HH}_2} P_{\text{HH}_2}}{r_{\text{HH}_2} + k_{\text{HH}_2} \sum_i b_{\text{HH}_2 i} \sum_j b_{\text{HH}_2 j}}, \quad (6) $$

where $\sum_i b_{\text{HH}_2 i}$ are the sum of the rates of all possible desorption mechanisms for gH on gH₂ substrates.

3 NUMERICAL COMPARISON

In order to test the validity of H atoms encounter desorption mechanism, we compare results from RE models with the inclusion of gH and gH₂ encounter desorption mechanism (hereafter REED) with these calculated by the microscopic MC approach. However, so far it is not possible to simulate a chemical model that includes H₂ accretion for any meaningful length of time using the microscopic MC method because the H₂ accretion and gH₂ hopping consume too much CPU time. Therefore, following Hincelin et al. (2015), we can only compare the steady-state gH abundances calculated by these two approaches. Moreover, we also adopt a simple chemical model which only considers the accretion of H and H₂, the thermal and encounter desorption of gH and gH₂ and the recombination of gH atoms on grain surfaces to form gH₂.

We adopt a typical dust grain with radius 0.1 μm. Such a grain has $S = 10^9$ binding sites. The desorption energies of gH₂ on water ice and gH₂ are assumed to be 440 K (Hincelin et al. 2015) and 23 K (Cuppen & Herbst 2007) respectively while the desorption energy of gH on water ice and gH₂ are assumed to be 450 K (Garrod & Herbst 2006) and 45 K (Cuppen & Herbst 2007) respectively. The diffusion barriers are always set to be half of the desorption energy for all surface species. Both the gas and dust temperatures are assumed to 10 K in our simulations. We assume the density of H₂ to be constant in each simulation. We perform simulations using a wide range of H nuclei densities, which vary from $2 \times 10^4$ cm$^{-3}$ to $2 \times 10^{14}$ cm$^{-3}$. Because the fractional abundance of H is around $1.0 \times 10^{-4}$ in dense clouds (Chang et al. 2007), we assume the fractional abundance of H atoms is fixed to be $2.5 \times 10^{-4}$ for all H nuclei densities for simplicity. So, the accretion rate of H atom is,

$$ k_{\text{accH}} X(H) = 1.0 \times 10^{-4} k_{\text{accH}_2} X(H_2), \quad (8) $$

where $k_{\text{accH}_2}$ and $k_{\text{accH}}$ are the accretion rate coefficients of gas-phase H₂ and H respectively while $X(H_2)$ and $X(H)$ are the densities of these two species respectively. Moreover, in order for a preliminary study of the effect of the gH encounter desorption on the surface chemistry, we also use the RE approach to calculate another chemical model, which has all the above reactions other than the encounter desorption of gH atoms. Hereafter, this model is called the REED2 model.

We briefly introduce the microscopic MC approach as follows and refer to Chang et al. (2005) for details of this numerical method. Grain surface binding sites form a
$L \times L$ square lattice, where $L = \sqrt{S}$. When gas-phase species accrete on grains, they are randomly located into binding sites. At time $t$, a surface species $g$ either hop to a neighboring site or desorb after a waiting time,

$$\delta t = -\ln(X)/(b_I(t) + k_I(t)),$$

where $b_I(t)$ and $k_I(t)$ are the desorption and hopping rates of species $I$ at the time $t$ respectively while $X$ is a random number uniformly distributed in $(0, 1)$. If the site where species $I$ resides at the time $t$ is already occupied by $gH_2$, the value of $b_I(t)$ should be the desorption rate of the species $I$ on $gH_2$. Otherwise, it is the desorption rate of species $I$ on water ice. Similarly, the value of $k_I(t)$ depends on whether the binding site is occupied by $gH_2$ or not. The species $I$ hops into a neighboring site if $k_I(t) \geq Y(b_I(t) + k_I(t))$, where $Y$ is another random number uniformly distributed in $(0, 1)$. Otherwise it will desorb. A chemical reaction occurs if the species $I$ hops into a site and encounters a reactive species.

In the microscopic MC simulations, the initial $gH$ and $gH_2$ abundances are zero. As $H$ and $H_2$ accrete on the grain surface, $gH$ abundance initially increases and then fluctuates around its mean value after the steady-state has been reached. The average abundance of $gH$ between time $t_0$ and $t_1$, which are both after the steady-state has been reached, is

$$gH(t_0, t_1) = \frac{\sum_i i \Delta t_i}{t_1 - t_0},$$

where $\Delta t_i$ is the time interval during which the number of $gH$ atoms is $i$ and $\sum_i \Delta t_i = t_1 - t_0$. If $t_1 - t_0$ is sufficiently large, $gH$ converges to a value that is independent of $t_1, t_0$ nor $t_1 - t_0$. At the low H nuclei density ($\sim 10^{-6}$ cm$^{-3}$), $t_1 - t_0$ is a time period during which about 4000 H atoms accrete on grain surface so that $gH$ can converge. As the H nuclei densities increase, more H atoms are required to accrete during the time period $t_1 - t_0$ so that $gH$ converges because of the larger $gH$ population fluctuations. We use the converged $gH$ values to compare with the abundances of $gH$ predicted by RE approach.

As introduced earlier, hydrogen atoms can encounter $gH_2$ in two different ways. When a $gH$ atom hops into a site occupied by $gH_2$, the desorption and hopping rates of $gH$ significantly increase because of the significantly reduced desorption energy and diffusion barrier of $gH$ on $gH_2$. On the other hand, when a $gH_2$ molecule hops into a water binding site occupied by a $gH$ atom, the $gH$ atom cannot hop or desorb until the $gH_2$ molecule leaves the binding site in the microscopic MC simulations (Chang et al. 2007). After the $gH_2$ leaves the binding site, the $gH$ atom can hop or desorb, but its desorption energy and diffusion barrier are still those on water substrates. Therefore, the first scenario of $gH_2$ and $gH$ encounter must occur so that $gH$ desorb more quickly. If the second scenario occurs, $gH_2$ may also desorb more quickly on that site than on water ice because the desorption energy of $gH_2$ on $gH$ is much less than that on water ice (Cuppen & Herbst 2007). A surface reaction $gH + gH_2 \rightarrow gH + H_2$ can be included in the reaction network in the RE approach in order to take into account of this $gH_2$ molecules desorption process when they encounter $gH$ atoms. However, because $gH_2$ is much more abundant than $gH$, this event occurs much less frequently than the process $gH_2$ encounter other hydrogen molecules does. Therefore, in this work, we ignore this desorption process and assume that the desorption energy of $gH_2$ on $gH$ is the same as that on water ice. Thus, the reaction $gH + gH_2 \rightarrow gH + H_2$ is not included in the reaction network.

Figure 2 shows the steady-state $gH$ abundance as a function of $H_2$ density from the microscopic MC and REED models. It can be seen that the $gH$ abundances predicted by the REED models agree very well with the results from the microscopic MC model for a wide range of $H_2$ density between $10^4$ cm$^{-3}$ and $10^{12}$ cm$^{-3}$. At the density of $10^4$ cm$^{-3}$, $gH$ abundance predicted by the microscopic MC method is slightly higher than that from the REED model because of the “back diffusion” problem. When the abundances of reactive surface species are very low on grain surface, two species must visit around 3S binding sites in order to encounter each other (Lohmar & Krug 2006; Chang et al. 2006). So the reaction rates in the RE model are overestimated while the microscopic MC method already takes into account the back diffusion. At higher $H_2$ densities, surface $H_2$ density also increases so that the back diffusion problem becomes less significant (Chang et al. 2006). Thus, the REED model results agree better with the microscopic MC model results. However when the $H_2$ density is above $10^{13}$ cm$^{-3}$, the microscopic MC model predicts that hydrogen molecules occupy about 70 percent of the total number of grain surface binding sites (Hincelin et al. 2015). If $gH$ hops from one binding site to another, it is very likely that the second binding site is also occupied by $gH_2$. This possibility is not considered by the RE approach. Therefore, the discrepancy between the REED and microscopic model results increase as gas-phase $H_2$ abundance increases. At the highest $H_2$ density, the abundance of $gH$ from the REED model is about a factor of four larger than that from the microscopic MC model.

Figure 2 also shows the steady-state $gH$ abundance as a function of $H_2$ density for the REED2 model. We
can see that the gH encounter desorption mechanism can decrease gH abundance by about one order of magnitude for the simple reaction network. Grain surface reactions are dominated by hydrogenation reactions at 10 K, so the significant decrease of gH abundance may change the abundances of icy species in a much larger gas-grain chemical model. The effects of gH encounter desorption on the formation of surface species at 10 K in a larger chemical model will be presented in the next section.

We fix the fractional abundance of H atoms to be $10^{-4}$ in the above simulations, however, the fractional abundances of H atoms in astronomical sources may not be always around that value. In order to study how the fractional abundances of H may affect the validity of H atoms encounter desorption mechanism, we fix the H nuclei density to be $2 \times 10^6$ cm$^{-3}$ and simulate the REED and microscopic MC models using a wide range of H fractional abundances, which vary from $10^{-6}$ to 0.1. We found that the gH abundances predicted by the REED model fall within 50 percent of that by the microscopic MC model over the wide range of H fractional abundances. Therefore, the agreement of the REED model with the microscopic MC model results is not likely to be noticeably affected by the fractional abundance of H atoms.

4 EFFECTS OF H ATOMS ENCOUNTER DESORPTION ON THE COLD CORE CHEMISTRY

The encounter desorption mechanism is not likely to be important when grain temperatures are high enough so that almost all gH$_2$ molecules sublime because the encounter events would be few if gH$_2$ abundance is low. Therefore, we only study the effects of H atoms encounter desorption on cold core chemistry.

The full gas-grain chemical reaction network was adapted from Garrod et al. (2007) and updated based on KIDA (Hincelin et al. 2011), which has 654 species and 6210 chemical reactions. The reactive desorption mechanism is included in this reaction network. Its coefficient is set to be 0.01. Initially, all species are assumed to be in the gas phase. The initial low-metal elemental abundances are taken from Semenov et al. (2010). The effect of quantum tunneling for grain-surface species is not considered in this work (Katz et al. 1999).

The two-phase model is used in all simulations. We use a standard dust grain with radius 0.1 µm with surface binding site density $1.5 \times 10^{15}$ cm$^{-2}$. Both the grain and gas phase temperatures are set to 10 K and the density of H nuclei is $2 \times 10^4$ cm$^3$ in our models. The cosmic-ray ionization rate is $1.3 \times 10^{-17}$ s$^{-1}$ and the visual extinction is 10 mag. Similar to the simple reaction network discussed above, the desorption energies of gH on water ice and gH$_2$ are 450 K and 45 K respectively while the desorption energies of gH$_2$ on water ice and gH$_2$ are 440 and 23 K respectively. The ratio of the diffusion barrier of each surface species to its desorption energy is kept to be 0.5 in our models.

We simulate two chemical models. Model A includes the reaction gH$_2$ + gH$_2$ → H$_2$ + gH$_2$ but not the reaction gH + gH$_2$ → H + gH$_2$. In model B, the two reactions gH$_2$ + gH$_2$ → H$_2$ + gH$_2$ and gH + gH$_2$ → H + gH$_2$ are included in its reaction network. In total, there are 6211 and 6212 chemical reactions in models A and B respectively. Both models are calculated by the OSU gas-grain RE codes (Garrod & Herbst 2006).

Figure 3 shows the temporal evolution of gas-phase and surface H atom abundances predicted by models A and B.
is included in model B, gH abundance from model B is typically lower than from model A. It is interesting that at the time earlier than 10^5 yr, models A and B predict similar gH and H abundances, which can be explained as follows. At the early time, there are abundant O, C and N in the gas phase, so most gH atoms react with gO, gC and gN on the grain surface instead of encountering gH_2 molecules and desorbing. When O, C and N atoms are depleted in the gas phase, it becomes more difficult for gH to find these atoms on grain surface to recombine, so gH can encounter gH_2 molecules more frequently. As a result, the impact of gH encounter desorption becomes more significant. Thus, the discrepancy between the gH abundances predicted by these two models becomes larger. At the time later than 3 × 10^5 yr, however, gH abundances predicted by model B become closer to that by model A, which can be explained as follows. In Figure 3, after 3 × 10^5 yr, the gas-phase H atom abundances gradually increase with time in model B while its abundances decrease with time in model A. At the time 10^6 yr, gas-phase H abundance in model B is about a factor of 4 larger than that in model A. Because of the higher gas-phase H atom density in model B, more H atoms accrete on grains in model B than in model A after the time 3 × 10^5 yr. So, gH abundances in model B are closer to that in model A after the time 3 × 10^5 yr. The largest discrepancy between the gH abundances predicted by these two models is about one order of magnitude, which occurs at around the time 3 × 10^5 yr.

Figure 4 shows selected major surface species abundances as a function of time from models A and B. These species are all surface hydrogenated products. We can see that the production of water ice and gNH_3 are not much affected by the gH encounter desorption mechanism introduced in model B. However, after the time 10^5 yr, model B predicts lower gCH_3OH and gH_2CO abundances than model A does because gH atom abundances in model B are lower. The difference of the impact on surface species production may be explained by the reaction barriers of hydrogenation reactions. Hydrogenation reactions that form gH_2 and gNH_3 are barrierless, thus, the rate coefficients of these hydrogenation reactions are large enough so that even when the gH abundances decrease, almost all gO and gN atoms can still be hydrogenated to form water and gNH_3 respectively. On the other hand, not all gCO molecules can be hydrogenated because the hydrogenation reaction gH + gCO → gHCO has a barrier. So, when the encounter desorption is introduced in model B, less gCO can be hydrogenated, thus, less gCH_3OH and gH_2CO molecules are formed in model B. We can also see that although it is more difficult to hydrogenate gH_2CO to form gCH_3OH in model B, overall, the gH_2CO abundances are reduced by the gH encounter desorption mechanism. The abundance of another major surface species gCO in models A and B differ by a factor less than 3. The abundances of gCO predicted by model B is always higher than that by model A after the time 10^5 yr because it is easier to hydrogenate gCO in model A due to the higher gH atom abundances.

The abundances of minor surface species may be more strongly affected by the encounter desorption of gH. Figure 5 shows the temporal evolution of selected minor surface species abundances from models A and B. After 10^5 yr, the abundances of these surface species from model B can be more than one order of magnitude higher than the results from model A. The encounter desorption of gH reduces its abundance in model B, so it is more likely that gO, gN and gC atoms react with each other to form -O-O-, -C-C- or -C-N- chemical bonds instead of reacting with gH atoms in this model. Thus, more gH_2O_2, gO_3, and gHC_3N can be formed in this model than in model A.
The encounter desorption of $gH$ may also impact the abundances of gas-phase species. Figure 6 shows the temporal evolution of selected gaseous species abundances. If a gas-phase species is mainly produced in the gas phase, the $gH$ encounter desorption is unlikely to impact its abundance. For instance, $HC_3N$ is mainly synthesized in the gas phase, so its abundances predicted by models A and B are almost the same. On the other hand, methanol can hardly be produced in the gas-phase. Almost all gaseous methanol are formed via reactive desorption on grain surface. Therefore, $CH_3OH$ abundance from model B is much lower than those from model A after the time of $10^5$ yr because surface methanol can be more efficiently synthesized in model A. Both $H_2O_2$ and $H_2CO$ can be formed in the gas phase and via reaction desorption on grain surfaces. Consequently, the impact of the $gH$ encounter desorption on their abundances is less than that on methanol abundances, but more than that on $HC_3N$ abundances.

We also performed test simulations of the above two models at a higher $H$ nuclei density, $10^5$ cm$^{-3}$. Similarly, model B considers the $gH$ atom encounter desorption mechanism while model A does not. We found that there are also less $gCH_3OH$ and $gH_2CO$ molecules and more surface species such as $gO_3$ in model B at the higher density. On the other hand, discrepancy between species abundances in the two models becomes less significant at the higher $H$ nuclei density. For instance, the surface methanol abundances from the model B are no more than a factor of 5 lower than that from model A at the higher $H$ nuclei density while the discrepancy can be as much as one order of magnitude at the lower $H$ nuclei density. We explain the decrease of the impact of the $gH$ encounter desorption when the $H$ nuclei density increases as follows. At the higher $H$ nuclei density, more species that can react with $gH$ accrete on grain surfaces, so it is more likely that $gH$ atoms react with other surface species instead of desorbing. Consequently, the $gH$ encounter desorption mechanism affects grain surface chemistry less significantly at the higher $H$ nuclei densities.

5 CONCLUSIONS AND DISCUSSIONS

The significantly reduced desorption energy of hydrogen atoms when encountering hydrogen molecules on dust grains, namely the encounter desorption mechanism of hydrogen atoms, is investigated in this work. This process can be easily included in an astrochemical model by adding a new chemical reaction, $gH + gH_2 \rightarrow H + gH_2$ to the chemical reaction network. We derived the rate coefficient for this reaction. In order to test the validity of hydrogen atom encounter desorption mechanism, we simulated a simple chemical reaction network that includes the encounter desorption of $H$ atoms by the RE approach and calculated the steady-state surface $H$ atom abundances. The calculated $H$ atom abundances agree well with those predicted by the more rigorous microscopic MC method over a wide range of gas phase $H_2$ and $H$ densities. Thus, the hydrogen atom encounter desorption mechanism is a reasonable approach to take into account of the facile desorption of hydrogen atoms on substrates composed of hydrogen molecules and water ice.

We simulated two full gas-grain chemical models under standard physical conditions that pertain to dense cores to investigate the impact of $gH$ encounter desorption mechanism. The $gH$ encounter desorption mechanism is present in model B, but not in model A. We found that the $gH$ atom encounter desorption can affect grain surface chemistry in two ways. Firstly, it becomes more difficult for hydrogenation reactions with barriers to fire if the $gH$ atom encounter desorption mechanism is included in the chemical model. Thus, the abundances of surface species such as methanol drops in the model because surface reactions that produce these surface species have barriers. Secondly, $gO$, $gN$ and $gC$ atoms are more likely to react with each other instead of reacting with $gH$ atoms in a model that includes the $gH$ atom encounter desorption mechanism.

Our approach can be generalized to other cases in which the facile desorption of a surface species $gX$ on a substrate $gY$ other than water ice has to be considered. We can simply add one surface reaction, $gX + gY \rightarrow X + gY$ in the chemical reaction network. The rate coefficient for this reaction can be derived in the same way as that for $gH$ encounter desorption.
Initially, the gH$_2$ encounter desorption mechanism was suggested to solve the problem that the coverage of gH$_2$ is too high at low temperatures and high H nuclei densities. Our study shows that at the lower H nuclei density, the gH encounter desorption mechanism may affect the production of surface species significantly. On the other hand, the major advantage of this approach is that it is very simple and easy to be implemented in a chemical model. Thus, this mechanism could be adopted widely in astrochemical modeling.

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