Recombination efficiency of molecular hydrogen on interstellar grains–II. A numerical study

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Abstract. A knowledge of the recombination time on the grain surfaces has been a major obstacle in deciding the production rate of molecular hydrogen and other molecules in the interstellar medium. We present a numerical study to compute this time for molecular hydrogen for various cloud and grain parameters. We also find the time dependence, particularly when a grain is freshly injected into the system. Apart from the fact that the recombination times seem to be functions of the grain parameters such as the activation barrier energy, temperature etc, our result also shows the dependence on the number of sites in the grain S and the effective accretion rate per site a_s of atomic hydrogen. Simply put, the average time that a pair of atomic hydrogens will take to produce one molecular hydrogen depends on how heavily the grain is already populated by atomic and molecular hydrogens and how fast the hopping and desorption times are. We show that if we write the average recombination time as $T_r \sim S^\alpha/A_H$, where, A_H is the hopping rate, then α could be much greater than 1 for all astrophysically relevant accretion rates. Thus the average formation rate of H_2 is also dependent on the grain parameters, temperature and the accretion rate. We believe that our result will affect the overall rate of the formation of complex molecules such as methanol which require successive hydrogenation on the grain surfaces in the interstellar medium.

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1.   Introduction

It has long been suggested that the dust grains play a major role in the formation of molecular hydrogen in the interstellar medium (ISM) (Gould & Salpeter, 1963). Considerable studies were made since then to understand the real physical processes which are taking place both theoretically (e.g., Hollenbach, Werner & Salpeter, 1971; Takahashi, Matsuda & Nagaoka, 1999; Biham et al. 2001) as well as experimentally (e.g., Pirronello et al. 1997a,b, 1999). More recently, Biham et al. (2001), and Green et al. (2001) have computed H_2 production rate by physisorption. It was found that a significant production is possible in cooler ($\sim 10 - 25K$) clouds. Cazaux & Tielens (2002, 2004) use both physisorption and chemisorption, to demonstrate that H_2 production is possible at high temperatures ($\sim 200 - 400K$) also. The goal is to study the rate at which the H atoms combine together on the surface of the grains to form H_2 and then they are desorbed into the gas phase to react with other atoms. When compared with the average mass fractions of various molecular species obtained through gas phase reactions (see, Chakrabarti & Chakrabarti, 2000ab; Das et al. 2006), it was found that the observed abundances of more complex species, such as methanol, are much higher. It is possible that methanol as well as its precursors also have to be formed on grain surfaces through successive hydrogenation. Our finding for molecular hydrogen has thus important bearings on the formation of more complex molecules on grains. These molecules would, in turn, desorb into the gas phase and would be expected to produce more complex species such as amino acids in due course.

One of the most challenging problems is to determine the average rate at which the recombination of atomic hydrogen takes place on a grain surface. In theoretical investigations which are prevalent in the subject (See, Acharyya and Chakrabarti, 2005; hereafter Paper I; Acharyya, Chakrabarti and Chakrabarti, 2005; hereafter ACC05), the diffusion rate A_H (inverse of the diffusion time $T_d = 1/A_H$) is divided by S, the number of sites on the grain surface (e.g., Biham et al. 2001) to get the recombination rate. The argument for reducing the rate by a factor of S is this: on an average, there are $S^{1/2}$ number of sites in each direction of the grain. Since the hopping is random, it would take square of this, i.e., S number of hopping to reach a distance located at $S^{1/2}$ sites away, where, on an average, another H is available. Thus, the effective recombination rate was chosen to be A_H/S. It is an empirical factor and needs more careful treatment. In our present paper, we replace S by an 'unknown' quantity $S' = S^\alpha(t)$, where $\alpha(t)$ may be time dependent (if the grain and cloud parameters change) and it could also deviate from unity. Let $\alpha = \alpha_0$ when a steady state is reached. Higher the accretion rate, lesser should be the value of α_0 as the effective surface area S' ($t \to \infty$) gets smaller and smaller. The opposite is true for smaller accretion rates. In fact, in the limit, if the accretion rate

is so low, that a lone H sweeps around the grain several times to find another H, one would get $\alpha_0 > 1$ since the effective site number is higher than S. Using our simulation, we determine how the effective site number deviates from S, one way or the other when the accretion rate is varied. Our result is likely to have important consequences for the formation of other hydrogenated species, such as water, methanol on grain surfaces. This will be discussed elsewhere. Some preliminary results with steady state α_0 have been presented in Das et al. (2005) and Chakrabarti et al. (2006). In the current paper, we discuss the time and temperature dependence of $\alpha(t)$ and studied the cases for more varied astrophysically important accretion rates.

In the next Section, we present the modified typical equations which govern the molecular hydrogen production rate on a grain surface. Incorporating the *physical aspects* of these equations, we perform a numerical simulation to determine the numbers on the grains. In Section 2, we present the procedure for the simulation and in Section 3 we present the results for two types of commonly used grains, namely, olivine and amorphous carbon. We show how $\alpha(t)$ depends on time and how it settles into a number (generally, > 1) when steady state is reached. Finally, in Section 4, we present our concluding remarks.

2. Procedure of numerical simulation

The relevant equations which are generally solved on grain surfaces have been presented in Paper I (Eqs. 2a-d) and we do not repeat them here. However, for Monte-Carlo simulation we need to modify these equations. Since in our simulation we expect to get the rate of diffusion $(T_r(t) = S/A_H)$ of H exactly, we can *assume* that the recombination time at any instant t could be written in the form:

$$T_r(t) = S'/A_H, \qquad (1)$$

where, S' is an 'effective surface area' which we may be written as $S' = S^\alpha(t)$. Here, $\phi_H = F_H(1 - f_{grh} - f_{grh2})$. F_H is the accretion rate of H and $F_H = A < v > N_H$, A being the area of a grain, $< v >$ is the average velocity and N_H is the number density of H in the gas phase. Our goal would be to compute the steady state value $\alpha_0 = \alpha(t \to \infty)$ for various grains (type and size) at various accretion rates and grain temperatures and to check if $\alpha \sim 1$. Thus, instead of Eqs. 2a of Paper I, the actual governing equation for atomic hydrogen should be,

$$\frac{dn_H}{dt} = \phi_H - W_H n_H - 2(A_H/S^\alpha)n_H^2, \qquad (2a)$$

along with equation governing the rate of production of H_2 given by,

$$\frac{dn_{H2}}{dt} = \mu(A_H/S^\alpha)n_H^2 - W_{H2}n_{H2}, \qquad (2b)$$

where, A_H is the hopping rate given by $\nu \exp(-E_0/k_b T)$, W_H is the desorption co-efficient of hydrogen atom given by, $\nu \exp(-E_1/k_b T)$, W_{H2} is the desorption co-efficient of hydrogen molecule given by, $\nu \exp(-E_2/k_b T)$. Here, E_0 is the activation barrier energy for diffusion of H atom, E_1 is the activation barrier energy for desorption of H atom and E_2 is the activation barrier energy for desorption of H_2 molecule, ν is the vibrational frequency given by, $\nu = \frac{2sE_d}{\pi^2 m_H}$, n_H be the number of H atoms, and n_{H2} be the number of H_2 on a grain at time t, $s \sim 10^{14-16}$ is the surface density of sites on a grain, m_H is the mass of the H atom and E_d is the binding energy. The parameter μ represents the fraction of H_2 molecules that remains on the surface upon formation while $(1-\mu)$ fraction is desorbed due to the energy released in the recombination process. The H_2 production rate R_{H2} in the gas due to grain is then given by,

$$R_{H2} = (1 - \mu)(A_H/S^\alpha)n_H^2 + W_{H2}n_{H2}. \tag{3}$$

The values of the activation barrier energies E_0, E_1 and E_2 are taken from Katz et al. (1999) and are given by, $E_0 = 24.7$ meV, $E_1 = 32.1$ meV and $E_2 = 27.1$ meV for olivine and $E_0 = 44$ meV, $E_1 = 56.7$ meV and $E_2 = 46.7$ meV for amorphous carbon grains. For olivine, $\mu = 0.33$ and for amorphous carbon $\mu = 0.413$ was used.

For the sake of simplicity, we assume each grain to be square in shape having $S = n^2$ number of sites (square lattice). We use periodic boundary condition so that the lattice behaves like a closed surface. We anticipate that the result would be insensitive to the actual nature of the lattice when simulation is done for a long time. We use mono-layer on the grain surface. We choose the minimum time step to be $t_h = 1/A_H$, the hopping time and advance the global time by this step. If ϕ_H is the effective accretion rate (as defined above), after every time step, i.e., after every $1/A_H$ seconds, ϕ_H/A_H number of hydrogen atoms are dropped on the grain. If ϕ_H is too low so that $\phi_H/A_H < 1$, then, clearly, one H is dropped after every A_H/ϕ_H steps. The exact site at which one atom is dropped is obtained by a pair of random numbers $(R_x, R_y, R_x, R_y < 1)$ obtained by a random number generator. This pair would place the incoming hydrogen at (i, j)th grid, where, i and j are the nearest integers obtained using the Int function: $i = int(R_x * n + 0.5)$ and $j = int(R_y * n + 0.5)$. Each atom starts hopping with equal probability in all four directions. This was decided by another random number. When, during the hopping process, one atom enters a site which is already occupied by another atom, we assume that a molecule has been formed and increase the number of H_2 by unity. However, when the atom enters a site occupied by an H_2, another random number is generated to decide which one of the other nearest sites it is going to occupy.

Thermal evaporation of H and H_2 from a grain surface is handled in the following way. Since W_H is the desorption rate for H, one atom is supposed to be released to the gas phase after every $1/W_H$ seconds. We generate a random number R_t for every H present on the grain and release (at each time step, i.e., $1/A_H$ seconds) only those for which $R_t < W_H/A_H$. Similar procedure is followed for the evaporation of H_2 for which the criterion for evaporation was $R_t < W_{H2}/A_H$.

Due to spontaneous desorption, a factor of (1-μ) of n_{H2} is lost to the gas phase. Here too, a random number R_s is generated for each newly formed (within that time step) H_2 present on the grain. Those which satisfy $R_s < (1 - \mu)$ are removed to the gas phase.

We continue our simulation for more than 10^9s. After an initial transient period, n_H and n_{H2} reaches a quasi-steady state with some fluctuations. In a steady state, α_0 can be calculated using Eq. 2a, i.e.,

$$\alpha_0 = log(\frac{2A_H n_H^2}{\phi_H - W_H n_H})/log(S). \tag{4}$$

In this context, one important parameter β may be defined as the 'catalytic capacity' of a grain (Chakrabarti et al. 2006) which measures the efficiency of the *formation* of H_2 on that grain surface for a given pair of H residing on it. Let δN_{H_2} be the number of H_2 *formed* in δt time. Since two hydrogen atoms are required to create one H_2, the average rate of creation of one H_2 per pair of H atom would be given by,

$$< A_{H1} >= \frac{1}{2n_H} \frac{\delta N_{H_2}}{\delta t}. \tag{5a}$$

We identify the inverse of this rate with the average formation rate given by,

$$T_f(t) = S^{\beta(t)}/A_H. \tag{5b}$$

Thus,

$$S^\beta(t) = A_H/ < A_{H1} > . \tag{5c}$$

This yields $\beta(t)$ as a function of time as,

$$\beta = log(A_H/ < A_{H1} >)/log(S). \tag{6}$$

Here too we can define $\beta_0 = \beta(t \to \infty)$. Our goal would be to see if β_0 thus obtained actually varies with grain parameters, accretion rate and temperatures. Intuitively, it should. This is because, when the accretion rate is very low, finding a second H on the grain would be difficult and it can take several sweeps of the grain surface. Thus $\beta_0 > 1$ would be a possibility. On the other hand, when the rate is very high, many sites would be occupied and another H would be met along any direction and β_0 could come down to 1/2 or even less. Indeed, this is what we see as well. We have carried out the simulation with and without spontaneous desorption taken into account. In presence of the spontaneous desorption, we remove H_2 by generating a random number as soon as one H_2 is formed and checking if it is less or more compared to μ. If less, H_2 remains on the grain, else it is taken out to the gas phase. The detailed results are discussed in the next Section.

3. Results and discussions

Fig. 1 gives the variation of n_H and n_{H2} residing on the grain surface since the beginning of the simulation. We chose a grain with 10^4 sites at 8K. For clarity, we plot average
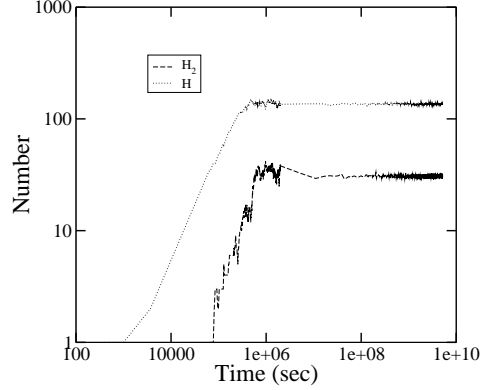
Figure 1. Variation of the number of H and H_2 on an olivine grain of 10^4 sites kept at 8K and exposed to an effective accretion rate per site of H 7.98×10^{-8} s^{-1}. We carried out our simulation near about 10^{10}s. For cleanliness, after the initial transient period of about 2×10^6s is over, we took time average at every 5.5×10^6s before plotting the numbers.

numbers in every $\sim 5.5 \times 10^6$s bin after the initial transient period of $\sim 2 \times 10^6$s is over. The simulation was carried out near about 10^{10}s. The effective accretion rate is assumed to be $\phi_H = 7.98 \times 10^{-4}$s^{-1}. In this case, the steady state has clearly been reached by this time and we can compute α_0 by using Eq. 4. This is done below.

3.1 Olivine grains

We start with the olivine grains which are kept at 8 K. The evaporation rate of H_2 is $W_{H_2} = 0.834844 \times 10^{-5}$ s^{-1} which corresponds to a time scale of ~ 119782.8s and similarly the evaporation rate of H is $W_H = 0.59 \times 10^{-8}$s^{-1} which corresponds to ~ 169585908s. The hopping time for hydrogen on this grain is 3680.58s (data taken from Katz et al. 1999).

In Fig. 2a, we present the computed α_0 (Eq. 4) as a function of a_s – the effective accretion rate per site. The solid, dot-dashed and the dashed curves are for $S = 10^4$, 9×10^4 and for 10^6 sites respectively. No spontaneous desorption has been included (i.e., $\mu = 1$). We extrapolated our curve to very low accretion rates which would have taken a very long computation time, just to show the trend of the result and extreme conditions. We note that α_0 is generally higher than unity in the region of our interest. This is because Hs are scattered few and far between and it takes a longer time (generally more than one sweeping) for one H to locate another. α_0 monotonically drops as the accretion rate goes up. In Fig. 2b, we show the variation of β_0 (Eq. 6) for the same case. Here too, we see that β_0 is very high compared to unity for low rates, but becomes ~ 0.5 or lower
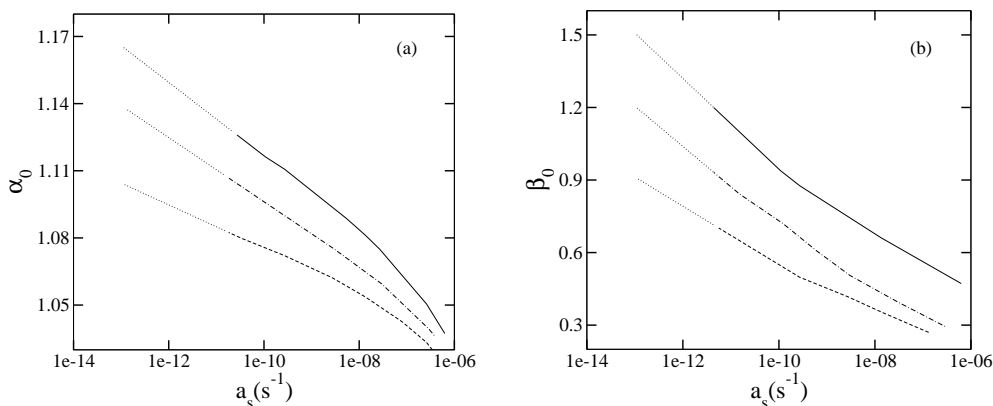
Figure 2. (a-b): Variation of (a) α_0 and (b) β_0 as a function of a_s, the effective accretion rate per site for various olivine grains kept at 8K. The dashed, dot-dashed and solid curves are for $S = 10^6$, 9×10^4, and 10^4 respectively. α_0 is clearly a function of the accretion rate. For rates relevant in molecular clouds α_0 and β_0 are much larger than unity. For very high rates β_0 comes down to 0.5 or lower. The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.

for higher rates as expected. Note that α_0 and β_0 go down with increasing site number S also. Since for a smaller grain, the possibility of getting it filled at a high rate is higher, one would have expected an opposite result. However, it is to be remembered that for a larger grain, the accretion rate itself ($\phi_H = Sa_s$) is also large. Hence the plots are to be compared carefully. For instance, the result of $a_s = 0.0005 \times 10^{-8}s^{-1}$ for 9×10^4 sites is to be compared with that of $a_s = 0.0045 \times 10^{-8}s^{-1}$ for 10^4 sites in order to make a meaningful comparison. In any case, for reasonable ϕ_H values with number densities up to 10^6 cm^{-3}, the relevant a_s would be below 10^{-6} where $\alpha_0 > 1$ in general.

In Fig. 3(a-b), we present snapshots of the occupancy of H (hollow squares) and H_2 (filled squares) at two instants of time on the grain containing only 900 sites at two arbitrarily chosen times (a) t=8×10^8s (b) t=10^9s respectively. Here an olivine grain at (8K) with 900 sites has been chosen. This grain is facing an accretion rate of F_H/S of 3.02×10^{-7}s^{-1} per site. No spontaneous desorption has been assumed here. This is to be compared with Fig. 3(c-d) for the same simulation and for the same time as before when the spontaneous desorption has been included. The numbers of H_2 are fewer since after formation of H_2 molecules some part of the H_2 are spontaneously desorbed in to the gas phase.

When temperatures of the grain is increased, all the rates go down exponentially. As a result, we expect α_0 to rise with temperature for a given accretion rate. In Fig. 4 we show this behaviour for $T = 8$, 9, 10K respectively for olivine grains. We choose $S = 10^4$
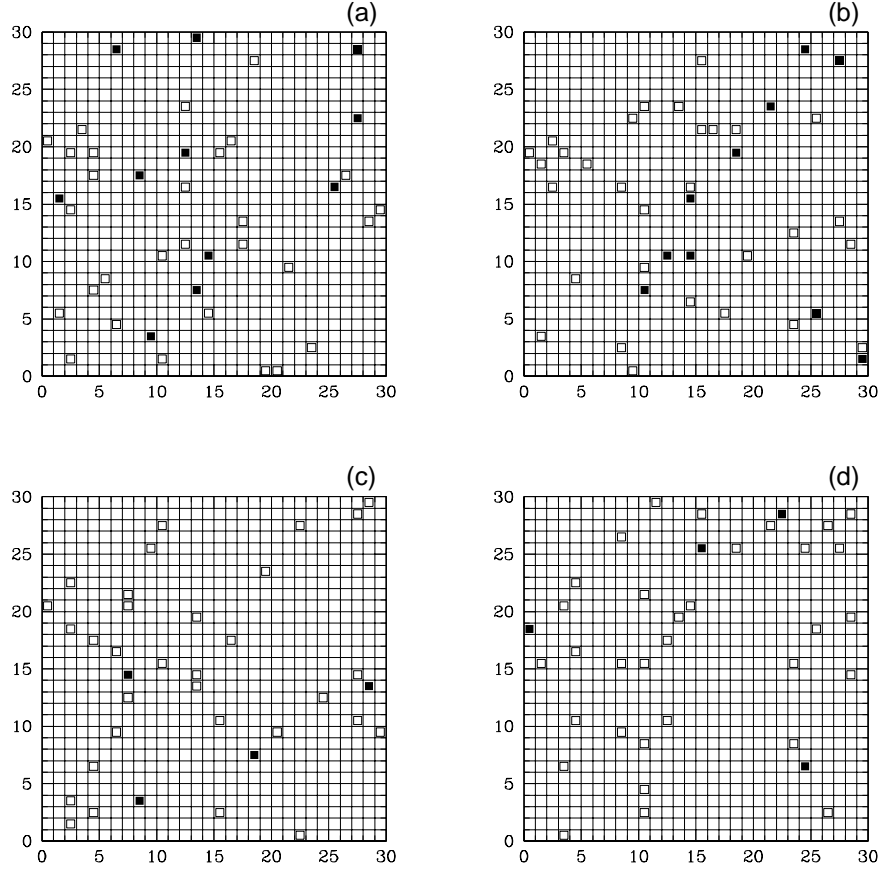
Figure 3. (a-d): In (a-b) snapshots of the grain surface with H (hollow squares) and H_2 (filled squares) at two arbitrarily chosen times (a) 8×10^8s and at (b)10^9s. Here an olivine grain (at 8K) with 900 sites has been chosen. This is bombarded with an accretion rate per site of H 3.02×10^{-7} per sec. No spontaneous desorption has been assumed here. In (c-d) spontaneous desorption has been included and plotted for the same time as before. Thus, numbers of H_2 residing on the grain at any instant are lesser.

in this case. This behaviour affects the recombination efficiency η as defined by,

$$\eta = \frac{2R_{H_2}}{F_H} \tag{7}$$

itself. In Fig. 5, we compare the temperature dependence of η as obtained from the rate equations (solid) curve with that obtained from our simulations. The accretion rate per site of 1.8×10^{-9} sec^{-1} was used (same in both the cases). We note that for $T \leq 7.5$K the simulation results are higher and for $T \geq 7.5$K the simulation results are lower. This
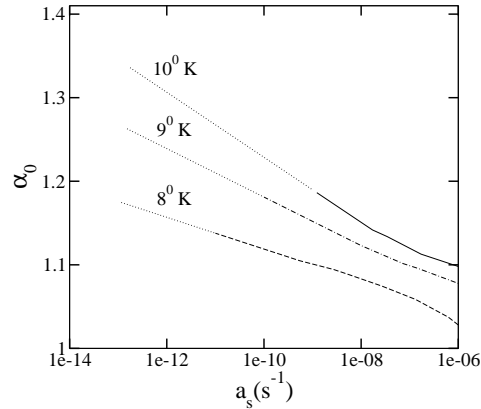
Figure 4. Temperature dependence of α_0 for the olivine grains at 10K (solid), 9K (dot-dashed) and 8K (dashed). The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.
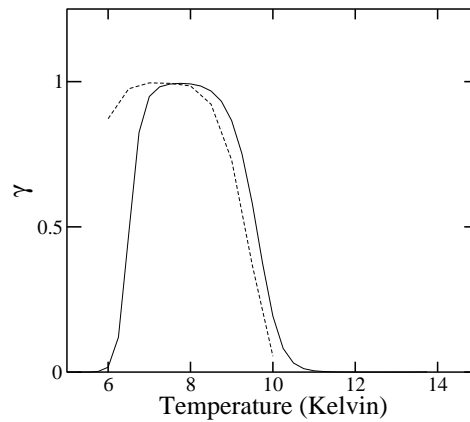
Figure 5. A comparison between the recombination efficiency obtained from the rate equation (solid) and that obtained from our simulation (dashed). We use the accretion rate per site 1.8×10^{-9} per second for a grain of diameter 0.1μm. The difference can be attributed to the temperature dependence of the α_0 as shown in Fig. 4 above.

is because α_0 itself is strongly temperature dependent as shown in Fig. 4 while the rate equation uses $S = S'$ (i.e., $\alpha_0 = 1$) for all temperatures.

In Fig. 6 we compare our results with the analytically obtained results from the rate equation method provided correct S' was chosen (Eqs. 2ab). The simulation results
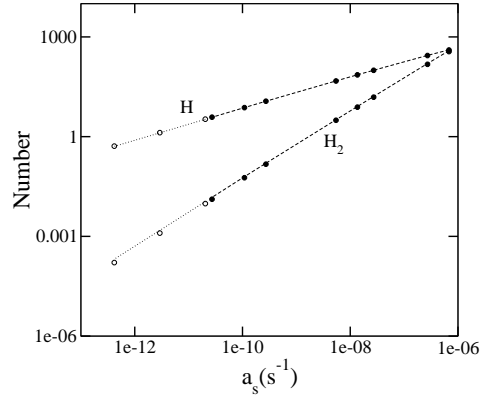
Figure 6. A comparison of the simulation results (dark circles) with those obtained from analytical considerations (dashed curves) when suitable modification of the average recombination rate is made. An olivine grain of 10^4 sites at a temperature of 8K has been chosen in this comparison. Dotted curves are drawn using analytical results for α_0 extrapolated to very low accretion rates.

are shown by the dark circles and those obtained from the analytical considerations are shown by the dashed curves. An Olivine grain of 10^4 sites at a temperature of 8K has been chosen in this comparison. Dotted curves are drawn using analytical results for α_0 extrapolated to very low accretion rates.

It is interesting to compare the results of our simulation with those obtained from the analytical considerations with and without our α_0 factor. In Table 1, we present this comparison. We take an olivine grain of 10^4 sites at 8K and vary the accretion rates. In Column 1, we give the accretion rate per site of the grain. In Column 2 we present the coefficient α_0 which we derive from our simulation. In Columns 3-5, we present the number of H as obtained by our simulation and the modified equation (Eq. 2a) and the standard equations (Paper I) respectively. Columns 6-8, we present similar results for H_2. We find that our simulation matches more accurately with the analytical results provided S' is chosen as the surface area. If the standard equation is used, the deviation is very significant. Indeed, the number of H on the grain could be roughly half as much when simplistic analytical model is used. What observe is that on the grains we tend to have more H and less H_2 than what analytical work suggests.
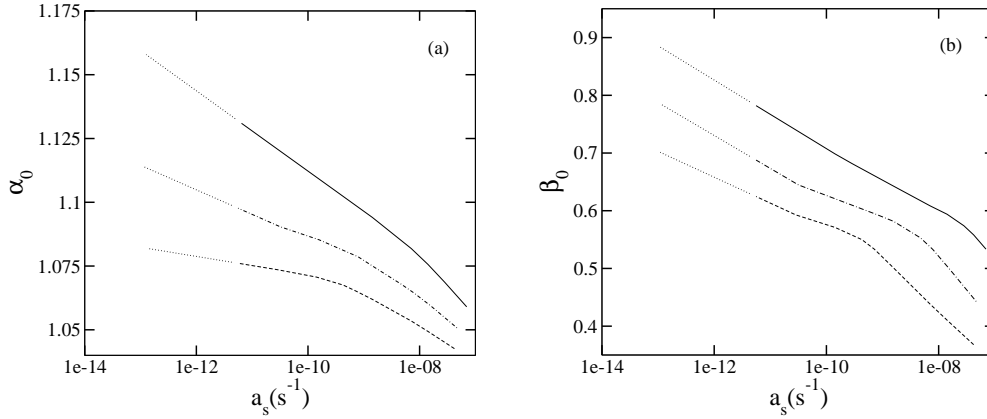
3.2   Amorphous carbon grains

Carbon grains produce significant H_2 at a higher temperature than olivine grains because all the barrier energies are higher. We plot in Fig. 7a the variation of α_0 with a_s at

Table 1. Comparison of H and H_2 abundances in various methods.

Accretion Rate per site $A_s(S^{-1})$	α_0	H with			H_2 with		
		simulation	$\alpha_0 \neq 1$	$\alpha_0 = 1$	simulation	$\alpha_0 \neq 1$	$\alpha_0 = 1$
6.79×10^{-7}	1.04	403.11	407.80	340.57	361.71	383.82	377.48
2.72×10^{-7}	1.05	275.78	278.02	219.31	149.96	158.16	156.53
2.72×10^{-8}	1.07	99.03	99.31	70.35	15.40	16.14	16.11
1.36×10^{-8}	1.08	72.27	72.42	49.80	7.71	8.08	8.07
5.43×10^{-9}	1.09	47.30	47.37	31.52	3.11	3.23	3.23
2.72×10^{-10}	1.11	11.62	11.62	7.01	1.49×10^{-1}	1.59×10^{-1}	1.60×10^{-1}
1.09×10^{-10}	1.12	7.46	7.48	4.42	5.81×10^{-2}	6.24×10^{-2}	6.35×10^{-2}
2.72×10^{-11}	1.13	3.86	3.82	2.18	1.31×10^{-2}	1.49×10^{-2}	1.55×10^{-2}
$*2.04 \times 10^{-11}$	1.13	3.36	3.33	1.89	9.7×10^{-3}	1.11×10^{-2}	1.17×10^{-2}
$*2.92 \times 10^{-12}$	1.14	1.32	1.30	0.70	1.3×10^{-3}	1.5×10^{-3}	1.6×10^{-3}
$*4.16 \times 10^{-13}$	1.16	0.52	0.51	0.26	2.00×10^{-4}	2.00×10^{-4}	2.00×10^{-4}
$*5.95 \times 10^{-14}$	1.17	0.20	0.20	0.10	2.11×10^{-5}	2.81×10^{-5}	3.13×10^{-5}

$*$ represents the extrapolated value.

Figure 7. (a-b): Variation of (a) α_0 and (b) β_0 as a function of a_s, the effective accretion rate per site, for various amorphous carbon grains kept at 14K. The solid, dot-dashed and dashed curves are for $S = 10^4$, 9×10^4, 10^6 respectively. The exponents α_0 and β_0 are strong functions of the accretion rate. For low rates β_0 is higher than unity, while for higher rates it is close to 0.5 or even lower. The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.

temperature 14K. The nature of variation of α_0 remains the same, namely, α_0 goes down with a_s. The solid, dot-dashed and the dashed curves are for $S = 10^6$, 9×10^4 and for 10^4 sites respectively. In Fig. 7b, we show the variation of β_0 and as expected its value can become as low as 0.5 for very large accretion rate. These results are representative as they are strongly temperature dependent as in the case of olivine (see, Fig. 4).

4. Concluding remarks

In this paper, we studied the behaviour of the average recombination time of atomic hydrogens on grain surfaces as a function of time, temperature, accretion rate and grain parameters. In the literature, it is simply assumed that the recombination time is grain site number divided by the diffusion rate. However, we find that this simplistic assumption is not valid especially when the accretion rate of H on the grain is very low or very high. For very low rates, an atomic hydrogen may have to sweep a grain several times before meeting another atom to form a molecule. For very high rates, the grain surfaces could be partially filled with H and H_2 and search for another H need not take S number of hops. We found that on an average, α_0, the index which determines the average recombination time, could be grater than 1 for very low rates. We also find that α_0 depends very strongly on the nature of the grains as well as the temperature and grain site numbers. We show how the number of H and H_2 change with time and determine the time scales in which quasi-equilibrium is reached. Thus the recombination time is a complex function of these parameters. We defined another index β (Chakrabarti et al. 2006) which is a measure of the average formation rate of H_2. This index also is also a strong function of accretion rate per site. In fact, for very high rates the index may go down to 0.5 or even lower. A comparison of the recombination efficiency as obtained from our procedure with that obtained from the rate equation clearly shows a deviation easily attributable to the temperature dependence of α_0 in a realistic case.

The results we obtained are likely to be astrophysically important because of several factors. The physical reason of the dependence of the average recombination time is so generic that one needs to revise all the abundances made on the grain surfaces. We find that even for H, we have more H left over on grains, while less H_2 is produced and released. Thus, analytical considerations will always over produce molecules obtained on grain surfaces. Similarly, if, for example, methanols are produced through successive hydrogenation process on a grain surface, at each step such corrections would be required and the final abundance would be greatly affected. This will be done in near future.

References

Acharyya, K., Chakrabarti, S.K., 2005, *BASI*, **33**, 473.
Acharyya, K., Chakrabarti, S.K., Chakrabarti, S. 2005, *MNRAS*, **361**, 550.
Biham, O., Furman, I., Pirronello, V., Vidali, G., 2001, *ApJ*, **553**, 595.
Cazaux, S., Tielens, A.G.G.M., 2002, *ApJ*, **575**, L29.
Cazaux, S., Tielens, A.G.G.M., 2004, *ApJ*, **604**, 222.
Chakrabarti, S., Chakrabarti, S.K., 2000a, *A&A*, **354**, L6.

Chakrabarti, S.K., Chakrabarti, S., 2000b, *Ind. J. Phys.*, **74B**, 97.

Chakrabarti, S.K., Das A., Acharyya, K., Chakrabarti, S., 2006, *A&A*, (in press).

Das, A., Chakrabarti, S.K., Acharyya, K., Chakrabarti, S., 2006, *A&A*, (submitted).

Das, A., Chakrabarti, S.K., Chakrabarti, S., Acharyya, K., 2005, *BASI*, **33**, 390.

Gould, R. J., Salpeter, E. E., 1963, *ApJ* **138**, 393

Green, N.J.B, Toniazzo, T., Pilling, M.J., Ruffle, D.P., Bell, N., Hartquist, T.W. 2001, *A&A*, **375**, 1111.

Hollenbach, D., Werner, M.W., Salpeter, E. E., 1971, *ApJ*, **163**, 165.

Katz, N., Furmann, I., Biham, O., Pironello, V., Vidali, G., 1999, *ApJ*, **522**, 305.

Pirronello, V., Liu, C., Shena, L., Vidali, G., 1997a, *ApJ*, **475**, 69.

Pirronello, V., Biham, O., Liu, C. Shena, L., Vidali, G., 1997b, *ApJ*, **483**, 131.

Pirronello, V., Liu, C., Riser, J.E., Vidali, G., 1999, *A&A*, **344**, 681.

Takahashi, J., Matsuda, K., Nagaoka, M., 1999, *ApJ*, **520**, 724.