ON THE FEASIBILITY OF DISK CHEMICAL MODELING

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Abstract. In this paper, we compare the results of the modeling of a protoplanetary disk chemical evolution obtained with the UMIST 95 and “New Standard Model” (NSM) chemical databases. Assuming the same initial conditions, it is found that the substitution of one chemical network by another causes almost no difference for the disk ionization degree. In contrast, the NSM and UMIST 95 abundances of CO can differ by a factor of a hundred at some regions of the disk surface. However, relevant CO vertical column densities differ much less, at most by a factor of a few. In addition, we synthesize the single-dish CO(J=3-2) line by means of the 2D line radiative transfer for both considered chemical networks. It is shown that the intensity of this line in the case of the UMIST 95 abundances is lower compared to the NSM case by \(\sim 15\%\).

Key words: astrochemistry – line: profiles – radiative transfer – planetary systems: protoplanetary disks

1. INTRODUCTION

Nowadays computational facilities allow to perform extensive simulations of the chemical evolution of various cosmic objects, like (collapsing) protostellar clouds or protoplanetary disks (e.g., Li et al. 2002; Aikawa et al. 2002). In these studies usually either the
UMIST 95 (Millar et al. 1997) or “New Standard Model” (Aikawa & Herbst 1999) database of chemical reactions is utilized. As the result of the modeling, time-dependent abundances of chemical species as well as their column densities can be obtained and faced with observational data. However, due to the lack of the full information about the physical conditions in the object under investigation and/or the complexity of the feasible modeling itself, typically these values are calculated with a certain (unknown) degree of accuracy. Therefore, it would be very useful to estimate, even approximately, how high it could be. The primary goal of this study is to verify how sensitive are the computed molecular abundances in the case of a protoplanetary disk chemistry to the adopted set of chemical reactions. Second, if such a difference exists for a certain species, we find by means of the reduction technique which chemical reactions are responsible for that. Finally, we study how such an abundance difference may affect the results of line radiative transfer calculations using the 2D line radiative transfer code “URAN(IA)”.

2. DISK MODEL

2.1. Disk physics

We used essentially the same disk physical and chemical model as described in Semenov et al. (2004) (hereafter Paper I). Briefly, the 1+1D flared steady-state accretion disk model of D’Alessio et al. (1999) is adopted with a radius of 373 AU, accretion rate $\dot{M} = 10^{-7} M_\odot \, \text{yr}^{-1}$, and viscosity parameter $\alpha = 0.01$. The central star is assumed to be a classical T Tau star with an effective temperature $T_* = 4000$ K, mass $M_* = 0.5 M_\odot$, and radius $R_* = 2 R_\odot$. We took into account the illumination of the disk by the stellar UV radiation with the intensity $G_* = 10^4 G_0$ at 100 AU, where $G_0$ is the intensity of the mean interstellar UV field by Draine (1978) as well as interstellar UV radiation, but neglected stellar X-rays. The cosmic rays are considered as another ionizing source with $\zeta_0 = 1.3 \cdot 10^{-17} \, \text{s}^{-1}$ unattenuated ionization rate. To calculate the propagation of the UV radiation and cosmic rays through the disk, Eqs. (2)–(3) from the Paper I are used. We did not take into account ionization by the decay of radionucleides.
2.2. Chemical model

Contrary to Paper I, a gas-grain chemistry without surface reactions is considered. In addition to our model which is based on the UMIST 95 ratefile, we adopted the NSM network (Herbst, priv. communication). The latter was extended by a set of reactions of dissociative recombinations on neutral and negatively charged grains as well as grain charging processes. We added a reaction of the H$_2$ photodissociation from the NSM model to our UMIST 95 network with unattenuated rate $k_0 = 3.4 \cdot 10^{-11}$ cm$^3$s$^{-1}$. All the rest parameters of the chemical model from Semenov et al. (2004) were the same. As the initial abundances, we used the same set of the “low metals” abundances from Wiebe et al. (2003) for the entire disk.

3. RESULTS

With the disk physical model and two chemical networks described in the previous section, we modeled the disk chemistry for 1 Myr evolutionary time span. The 2D disk distributions of the NSM-to-UMIST 95 ratio of the resulting fractional ionization and CO abundances are plotted in Figure 1, left and right panels, respectively. As clearly seen, there is no difference for disk ionization degree in the entire disk but one small region, $r \sim 350$ AU, $z \sim 235$ AU, where it can reach a factor of 200. On the contrary, $n_{\text{NSM}}(\text{CO})/n_{\text{UMIST}}(\text{CO}) > 1$ and can be as high as about 100 in the disk surface, $\log(z/Z) \sim -0.4$. However, the maximum CO gas-phase concentration is reached in the disk intermediate layer, $-1.0 < \log(z/Z) < -0.3$, where both the UMIST 95 and NSM networks give approximately the same values of the carbon monoxide abundances. Therefore, the corresponding
CO vertical column densities do not deviate much, at most by a factor of several for the disk inner and outer radii (see Figure 2, left panel). Using the UMIST 95 and NSM disk abundances of CO, we synthesized the single-dish CO(3-2) spectra with the 2D line radiative transfer code “URAN(IA)” (Pavluchenkov et al. 2003), which are plotted in Figure 2, right panel. It can be clearly seen that the intensities of this line differ by about 15%, which is lower than typical 30%–50% uncertainty of the observational data.

To figure out what is the reason for the difference in CO disk abundances, we used the reduction technique from Wiebe et al. (2003) and isolated two small subsets of primary carbon monoxide formation and destruction routes for both chemical networks. Surprisingly, it is found that these two sets contain nearly the same chemical reactions but some of them differ by the adopted rate coefficient values. Among the reactions with different rates, we designated three most important ones, which are listed in Table 1. Note that the corresponding rate values are given for the disk location $r = 10$ AU, $z = 3.15$ AU, where gas temperature and particle density are $T = 143$ K and $n = 3.3 \cdot 10^7$ cm$^{-3}$, the UV intensity and visual extinction are $G_\ast = 9.1 \cdot 10^5$ and $A_V = 1.2^m$, and ionization rate is $\zeta = 7.45 \cdot 10^{-18}$ s$^{-1}$. 

Figure 2: The radial distribution of the CO vertical column densities is presented on the left panel. The solid line with filled circles corresponds to the case of the UMIST 95 database, while the dashed line with open squares is for the NSM chemical network. On the right panel, the synthetic single-dish CO(3-2) line profiles calculated with the UMIST 95 (solid line) and NSM (dotted line) abundances of CO are depicted. It is assumed that the disk has the distance of 150 pc, its inclination angle is $30^\circ$, and the beam size of the telescope is $10''$. 
Table 1. Chemical reactions which cause the most of the CO disk abundance difference.

| Reaction                  | UMIST 95 rate, cm$^3$s$^{-1}$ | NSM rate, cm$^3$s$^{-1}$ |
|---------------------------|-------------------------------|---------------------------|
| C$^+$ + OH → CO$^+$ + H   | $7.7 \cdot 10^{-10}$         | $8.3 \cdot 10^{-9}$       |
| CO$^+$ + H → CO + H$^+$   | $7.5 \cdot 10^{-10}$         | $9.0 \cdot 10^{-11}$      |
| CO + $h\nu$ → C + O      | $9.1 \cdot 10^{-6}$         | $1.4 \cdot 10^{-6}$       |

4. SUMMARY

The sensitivity of the results of the disk chemical modeling to the applied chemical databases is investigated. It is found that the modeled disk fractional ionizations are nearly identical for both the UMIST 95 and NSM networks, while the CO abundances can vary by a factor of a hundred in some parts of the disk. However, the corresponding vertical column densities of CO do not show such a strong variation with the adopted set of chemical reactions. Consequently, it results in a small (∼15%) difference between the synthetic single-dish CO(3-2) line intensities obtained with two considered chemical sets.

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