

Chemical Reactions and Dust Destruction in Protoplanetary Accretion Disks

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Abstract. A nonequilibrium calculation for the chemistry in a classical protoplanetary accretion disk is presented. Slow radial particle transport moves grains from the cold outer regions of a protoplanetary accretion disk into its warm central part where grains are destroyed. We consider the destruction processes for the silicate and carbon dust component and follow the chemical composition of the gas as a function of the radial distance from the protostar. The main result of this calculation is the presence of huge amounts of methane at a distance of ~ 1 AU from the protostar as product of the carbon dust destruction. It is very likely that more complex organics also are present in this region.

1. Introduction

Chemical processes (e.g., molecules and dust reactions) play an important role for the structure and evolution of protoplanetary accretion disks. The chemical reactions, together with dust formation and destruction, determine the abundance of the absorbers and, thus, the opacity of the mixture of gas and dust, and the gas temperature. Temperature changes due to opacity changes, in turn, influence the rates of the chemical processes and the further chemical evolution of the system. This interplay between chemistry, opacity and temperature is of crucial importance and decides about the stability or instability of the disk, i.e., decides whether a disk may exist at all. Currently, limit cycle instabilities are under discussion as possible causes for the luminosity variations of certain classes of variable stars.

2. Model assumptions

The evolution in time and space of accretion disks as well as their chemical evolution are of fundamental importance for understanding the formation of planetary systems in general, and of our Solar System in particular.

2.1. Gas phase chemistry

The evolution of the number density n_i of each species i is determined by the continuity equation

$$\partial_t n_i + \partial_{\vec{x}}(n_i \vec{v}) = R_i \quad (1)$$

(v : gas velocity). Turbulent diffusion in a viscous accretion disk is not yet taken into account. In the present model calculation the continuity equation is solved in a comoving reference frame. In this case the set of rate equations is reduced to a system of ordinary differential equations.

For the rate coefficients R_i we take into account binary reactions between gas phase species, some ternary reactions to allow for H_2 formation in the denser parts of the disk, and surface reactions with dust particles to allow for dust particle destruction and growth. The corresponding rate coefficients for the gas phase reactions are

$$R_i = \sum_{j,l} k_{ijl} n_j n_l \quad \text{and} \quad R_i = \sum_{j,l,m} k_{ijlm} n_j n_l n_m \quad (2)$$

The rate coefficients for gas phase reactions are approximated by the standard Arrhenius form

$$k = A T^\beta \exp(-T_0/T) \quad (3)$$

Currently, we consider only neutral-neutral reactions of ≈ 80 atomic and molecular species of the most abundant elements H, C, N, O, Mg, and Si, and ≈ 450 chemical reactions between these species. The chemical network is nearly identical with that given by Mitchell (1984). Several rate coefficients have been updated using data from Baulch *et al.* (1992).

Additional rate terms account for the injection of matter into the gas phase when ice mantles evaporate.

2.2. Evaporation of dust and ice

In order to investigate the evaporation of ice mantles and of dust particles we use the following model:

a) We assume that there exist two dust components: olivine and carbon dust. Initially all Si is bound in olivine and 70 % of the carbon is bound in carbon dust (with the remaining 30 % in the gas phase as CO) according to Mathis *et al.* (1977). Since the thermodynamical properties of olivine seem not to be known we treat this dust component as Mg_2SiO_4 .

b) At the disk's outer radius the temperatures are so low that – with the exception of H_2 , H and N_2 – all molecular species are frozen out, especially H_2O and CO. Less abundant species like CH_3OH , which are frozen into the ice mantles (Pollak *et al.* 1994) and are liberated during their vaporization, are presently not considered. We assume that the dust grains are coated by an outer mantle of CO ice and an inner mantle of H_2O ice. This neglects that some of the CO is bound into the H_2O ice (Sandford & Allamandola 1993).

c) Evaporation of carbon at ≈ 1500 K adds C_i molecules to the gas phase (mainly with $i = 1, 2, 3$). These undergo further reactions until they finally are transformed into CO. The corresponding reactions are part of our reaction network. Silicate dust is destroyed by evaporation above ≈ 1650 K. This mainly

adds SiO, O, and Mg to the gas phase. Details of our treatment of evaporation of dust particles are given in Duschl *et al.* (1996).

d) We assume a size distribution of the ensemble of dust particles as in Mathis *et al.* (1977). This does not agree well with the absorption properties of dust in star forming regions, where small particles seem to be less abundant than in the Mathis *et al.* model. The strong coupling between dust absorption and disk structure during the silicate vaporization depends, however, only on the disappearance of the large grains (see Duschl *et al.* 1996).

e) The process of evaporation of ice mantles and of dust is modelled by calculating the change of radius of the ice layers and the dust particles, taking properly into account the size distribution of dust grains.

2.3. Oxidation of carbon dust

The carbon dust can be eroded by chemical reactions with molecules from the gas phase. From flame chemistry it is known that the most efficient processes are oxidation by oxygen bearing molecular species, especially by OH and O₂ (El-Gamal 1995). The most promising process in the protoplanetary disk is oxidation by OH radicals. The essential first step is (El-Gamal 1995):



which releases two carbon atoms. The ketyl radical HCCO reacts in the gas phase according to



This converts one of the two carbon atoms immediately into CO. The subsequent reactions of the CH₂ radical are described later.

2.4. The disk model

Currently we describe the structure of the protoplanetary disk by a semi-analytical model in the approximation of a thin, viscous accretion disk. The pressure P , central plane temperature T , vertical thickness h , viscosity ν and inward drift velocity v_s are given in this model by (Duschl *et al.* 1996)

$$P = 71.65 s^{-\frac{51}{20}} \left(\frac{M}{M_\odot}\right)^{\frac{5}{8}} (M_{-7}\kappa)^{\frac{1}{8}} \left(\frac{1}{\mu}\right)^{\frac{1}{2}} \left[\frac{\text{g}}{\text{cm s}^2}\right] \quad (6)$$

$$T = 997 s^{-\frac{9}{10}} \left(\frac{M}{M_\odot}\right)^{\frac{1}{4}} (M_{-7}\kappa)^{\frac{1}{4}} \text{ [K]} \quad (7)$$

$$\nu = 2.867 \cdot 10^{14} s^{\frac{3}{5}} M_{-7} \left[\frac{\text{cm}^2}{\text{s}}\right] \quad (8)$$

$$h = 1.446 \cdot 10^{12} s^{\frac{21}{20}} \left(\frac{M}{M_\odot}\right)^{-\frac{3}{8}} (M_{-7}\kappa)^{\frac{1}{8}} \left(\frac{1}{\mu}\right)^{\frac{1}{2}} \text{ [cm]} \quad (9)$$

$$v_s = 26.94 s^{-\frac{2}{5}} M_{-7} \left[\frac{\text{cm}}{\text{s}}\right] \quad (10)$$

The symbols have the following meanings: s is the radial distance from the accreting object in AU, M is the mass of the central accreting object (the Protosun), M_\odot is the solar mass, M_{-7} is the accretion rate in units of $10^{-7} M_\odot/\text{yr}$,

κ is the mass absorption coefficient and μ is the mean molecular weight. The numbers correspond to an assumed surface mass density of 2500 g/cm^2 at 1 AU.

The dust opacity is calculated simultaneously with the chemical composition of the gas, the destruction processes for the dust grains, and the disk structure. The mass absorption coefficient of the dust is calculated from the model of Draine (1985). For simplicity, we currently assume that the mass absorption coefficient of the gas component is constant.

We prescribe the initial conditions for the chemistry at $s = 1000 \text{ AU}$ and solve the equations from this point inwards. The initial composition of the gas phase is assumed to be: 10^{-5} of the hydrogen as free atoms, the remaining fraction not bound into molecules is H_2 , all nitrogen is in N_2 . All carbon not bound in dust particles is in CO and all oxygen not bound in CO or dust is in H_2O . CO and H_2O are frozen out as ice mantles on the dust particles. Less abundant species may be present in the gas phase, in the dust grains or in their ice mantles (e.g., Pollack *et al.* 1994), but these are neglected because they are unlikely to be of importance for the chemistry in the warm inner regions of the disk. We use solar system abundances as given by Anders & Grevesse (1989).

We follow the chemical evolution in a gas element which moves from larger radii towards the center of the disk with velocity v_s . During this inward drift the temperature and pressure increases resulting in changes in the chemical composition of the gas phase and of the amounts of ices and dust present. The temperature is calculated at every time step self-consistently taking into account the calculated dust opacity and an approximation for the gas opacity.

This model results in an extremely stiff system of ordinary differential equations that is coupled with a set of strongly non-linear algebraic equations for the disk structure and opacity. For the integration of the system we use a multistep, variable order backward differentiation method described in Bauer *et al.* (1996).

3. Results and interpretation

Figure 1 shows the chemical composition of the gas phase in the disk's central plane in the radial range where the carbon and silicate dust is destroyed. At larger radii (not shown here) first CO ice evaporates at $\approx 21 \text{ AU}$ where $T \approx 30 \text{ K}$, and then water ice evaporates at $\approx 8 \text{ AU}$ where $T \approx 150 \text{ K}$. The first dust component to be destroyed is the carbon dust. Between 1 and 0.5 AU, in the temperature regime between $T \approx 1000$ and $\approx 1300 \text{ K}$ (see Fig. 3), the carbon is oxidized by OH radicals resulting ultimately in an increase of the CO abundance in the gas phase and a corresponding decrease of the water steam abundance. In principle, the carbon is destroyed in the protostellar disk by the process of water gas production which converts carbon into CO and H_2 .

The first steps of this process are the two reactions (4) and (5). The CH_2 resulting from reaction (5) reacts with molecular hydrogen to form CH_3 and CH_4



From several possible reaction paths from this to CO , the most efficient one in the protoplanetary disk according to the results of our model calculation seems to be the condensation reaction

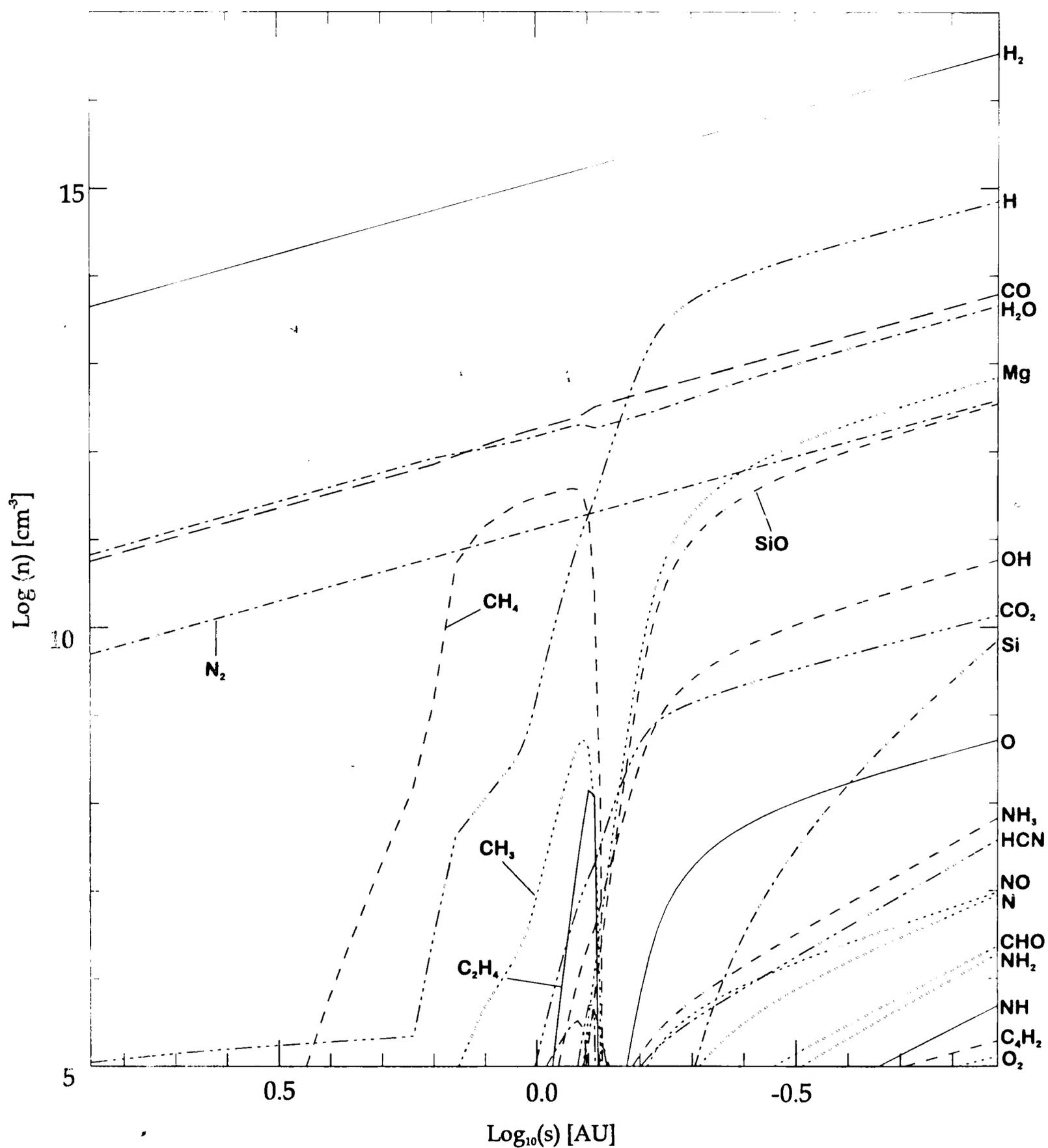
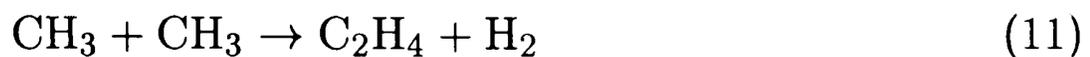
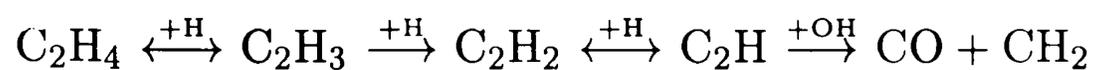


Figure 1. Chemical composition of the disk in the central plane



followed by



This sequence of reactions converts the second carbon atom released in reaction (4) into CO. The intermediate products CH_4 and CH_3 accumulate to considerable abundances in the gas phase (cf. Fig. 1) since reaction (11) becomes fast only if the abundance of CH_3 has increased to a sufficient level. This delays the conversion of the second carbon atom into CO to a temperature where already most of the carbon is gasified.

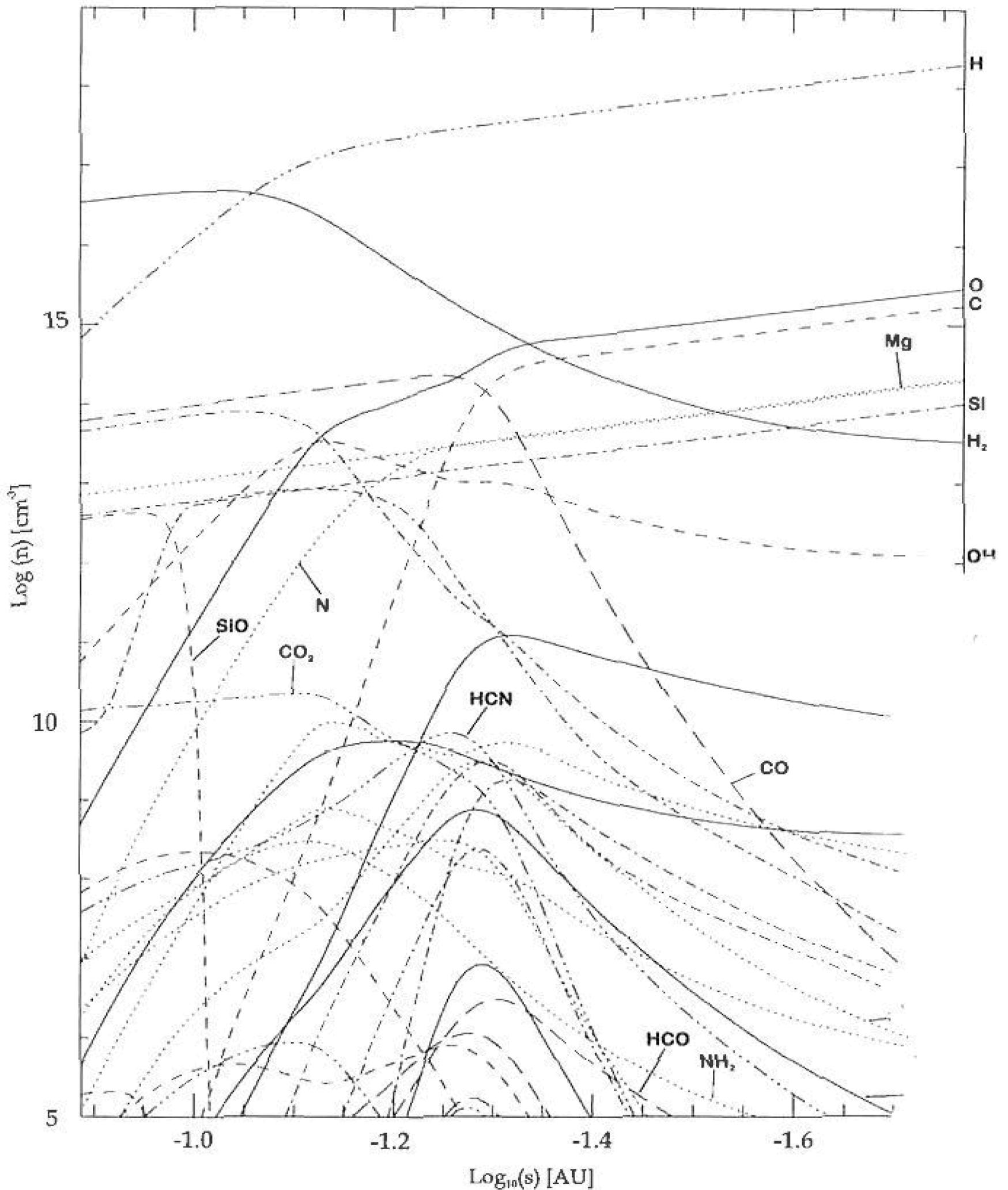


Figure 2. Chemical composition in the central plane of the disk: The region of CO dissociation.

An alternative path to CO would be reactions of CH_i molecules with OH to form HCO or H_2CO and from this CO. These reaction paths turn out to be inefficient in the protoplanetary disk.

Between 0.5 and 0.1 AU corresponding to the temperature regime 1650 ... 2100 K the olivine dust evaporates. This injects the decomposition products Mg, SiO, and O into the gas phase. SiO is dissociated by collision with H_2 and H. In our current calculations Si and Mg remain unchanged

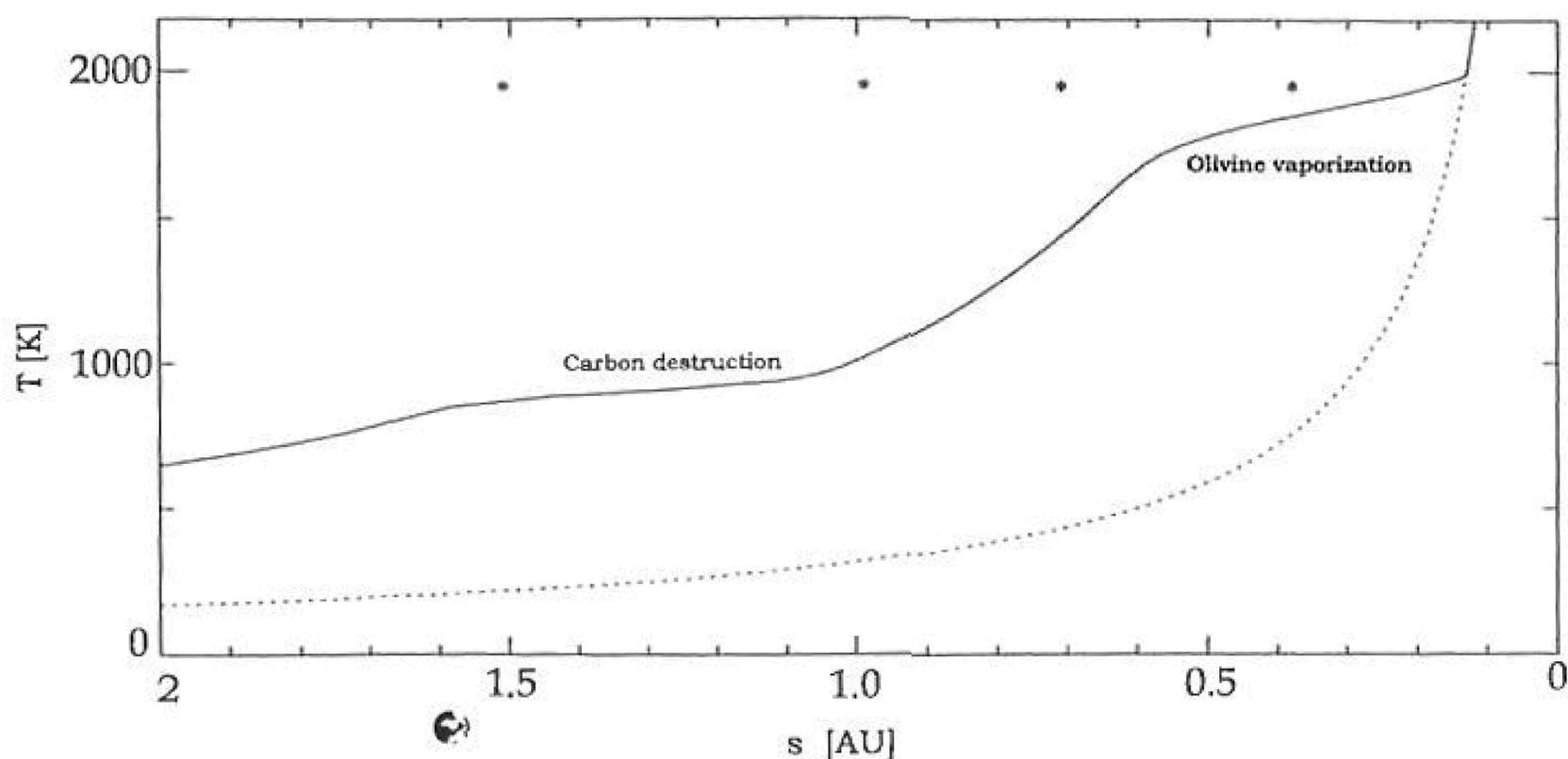


Figure 3. Temperature in the central plane of the protoplanetary disk

rise because no reactions of these species are taken into account. The gas released by silicate decomposition forms H_2O .

Figure 2 shows an enlargement of the inner part of the disk where a huge amount of new molecular species occurs, especially carbon compounds. This is due to the fact that part of the carbon is liberated by CO dissociation. Most molecules dissociate for radii $s < 0.06$ AU. Dissociation of molecular carbon occurs at $s \approx 0.09$ AU. Close to the center of the disk only the free atoms C, N, O, Mg, and Si remain.

As a direct consequence of the oxidation process for carbon dust, we obtain large amounts of methane in the disk between 1.4 and 0.8 AU i.e. *where the terrestrial planets are presently located*. The earth is located in the middle part of this region. This means that the earth has formed in an environment where large amounts of organic molecules were present. We expect that additionally many more complex organic molecules are formed in this region, as well, but these molecules are not yet implemented in the present simulation. The carbon oxidation by HCCO formation in the surface reaction (4) is the key process leading to these huge amounts of methane. A test calculation which omits the oxidation leads to small amounts of methane and organics only.

It is interesting to compare the central plane temperature for two models: one with and one without considering dust opacities, see Fig. 3. The dotted line corresponds to a model without dust opacity (i.e. only with an estimated gas absorption coefficient of $0.01 \text{ cm}^2/\text{g}$). The temperature in a model with dust opacity (full line in Fig. 3) shows two plateaus corresponding to the evaporation of carbon (1 - 0.5 AU) and of olivine (0.5 - 0.1 AU). The plateaus are due to the increase of opacity during dust destruction which counteracts a temperature increase with decreasing distance. The two curves merge where the last dust grains disappear.

Figure 4 shows the thickness of the accretion disk. The reduction of the disk thickness with decreasing absorption can be clearly seen. The figure additionally

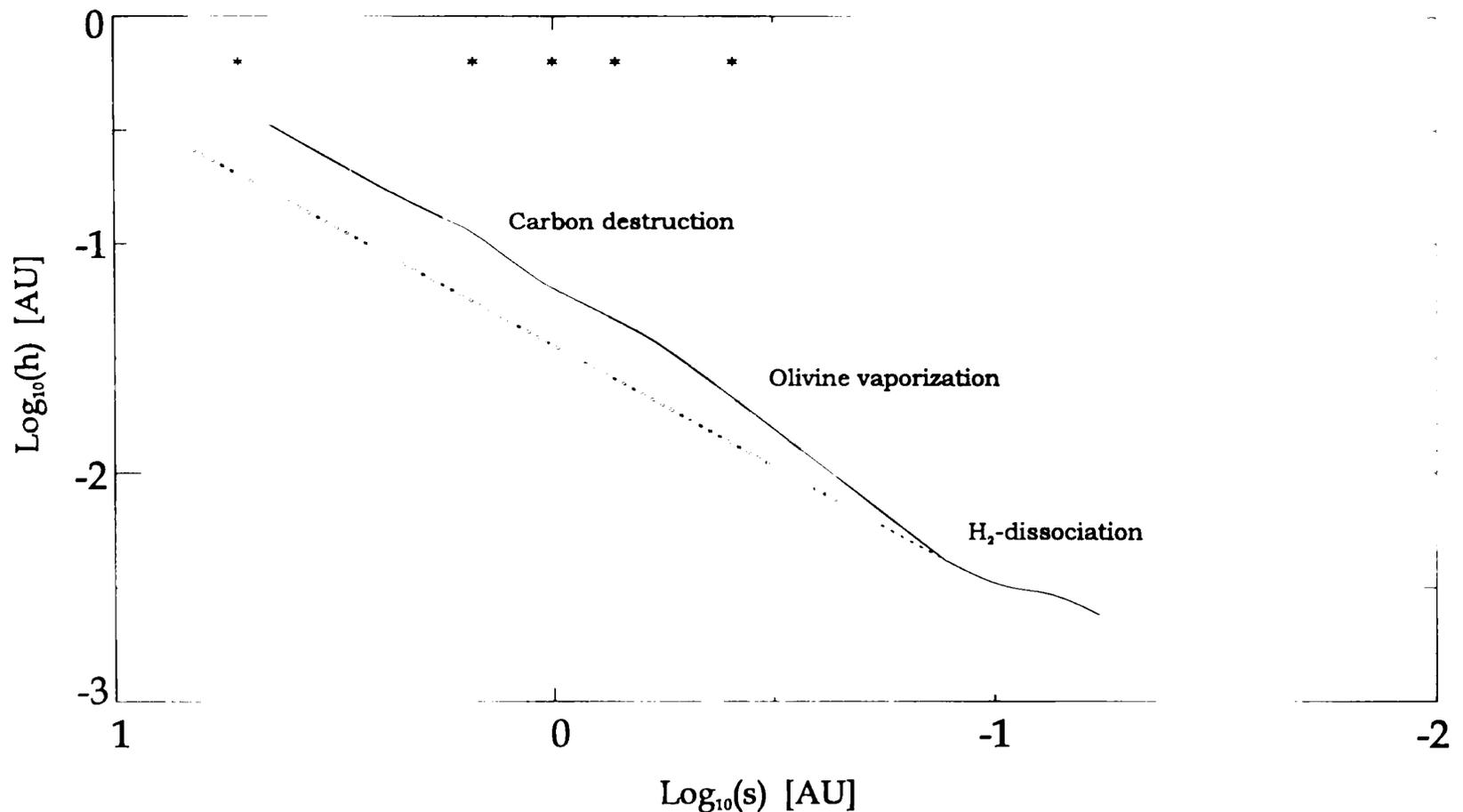


Figure 4. Thickness of the protoplanetary accretion disk

shows a short plateau in the disk around $s=0.05$ AU where H_2 dissociates. The increasing particle density in this region prevents the further shrinkage of the disk over a short radius interval.

The asterisks in Figs. 3 and 4 indicate the present positions of the planets from Jupiter to Mercury.

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