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Interaction between gas and ice phase in the three periods of the solar nebula

Carmen Tornow[1], **Ekkehard Kührt**[1], **Stefan Kupper**[1], **and Uwe Motschmann**[2]

[1]Inst. of Planetary Research,
Rutherfordstr. 2, D-12489 Berlin, Germany
email: carmen.tornow@dlr.de,ekkehard.kuehrt@dlr.de, and stefan.kupper@dlr.de

[2]Inst. of Theoretical Physics, Technical University Braunschweig,
Mendelssohnstr. 3, D-38106 Braunschweig
email: u.motschmann@tu-braunschweig.de

Abstract. We simulate the chemical processes in the three evolution periods of the solar nebula, which are (i) the quasi-stationary prestellar cloud core, (ii) the gravitationally collapsing protostellar core, and (iii) the evolving gas-dust disk. Our purpose is to identify chemical parameters which reflect special aspects of the interactions between the gas and ice phase in the different periods, e.g. isotopic or molecular ratios. In this study we derive the D/H and $^{15}N/^{14}N$ ratio of selected compounds as well as the CO_2/H_2O ratio to measure the fraction of non-polar to polar ice in the grain mantles. The chosen ratios depend on the depletion-enrichment relation between the ice and gas phases driven by the thermal evolution in each period, especially during the collapse. Hence, we have made great efforts in order to derive realistic and compact hydrodynamic models to describe the evolutionary periods of the solar nebula.

Keywords. Astrochemistry, star formation, comets, hydrodynamics, molecular processes

1. Introduction

Stars form from gas clumps with a small dust amount ($\approx$1% in mass) which are density fluctuations on an extended size range of a large turbulent hydrogen cloud. We assume that this was true for our sun as well. In the following sections we will describe each evolution period of the solar nebula in more detail and calculate the time dependency of its chemical composition in the gas and ice phase. The complete time interval of the three different periods of the solar nebula extends over about 40 million years. The chemical evolution is studied by means of ratios defined for selected species. At the beginning of the simulation process the gas phase contains 321 different species denoted by $x(\mathrm{i})$ and the ice phase is formed from 50 compounds symbolised by $x^*(\mathrm{i})$. The isotope ratios are derived from water and HCN in the case of the D/H ratio and from N_2H^+ for the $^{15}N/^{14}N$ ratio. Note, that the latter is a gas phase ion, since the ^{15}N chemistry is not contained in our ice phase model so far. The polar to non-polar ice fraction is measured by $x^*(CO_2)/x^*(H_2O)$ where H_2O and CO_2 are major species of the interstellar and cometary ice.

Essentially, one could propose more complex ratios in order to measure the corresponding material fractions, but due to feasibility restrictions in modelling methods and the amount of available observational results of ice phase abundancies for a future verification of our results we have considered simple and commonly occurring molecules, especially in comets. Since they consists of relatively pristine material the comets can be seen as important representatives for the ice phase of the solar nebula.

2. Simulation of the quasi-stationary prestellar cloud core

The quasi-stationary evolution of a prestellar core is modelled with a linear time dependency of the temperature and density. Systematic flow processes are not considered. The negligence of flows and unsteady evolution events such as shock waves or cloud collisions is justified since the temperature and density of the cloud core change over the large time interval of nearly 30 million years. The initial and final temperature and density at the beginning and end of the evolution interval are given by

$$T_{init} = 70\,\mathrm{K} \quad and \quad \rho_{init} = 3.1 \times 10^{-21} g/cm^3 \quad \text{for} \quad t = 0$$

$$T_{final} = 10\,K \quad and \quad \rho_{final} = 1.8 \times 10^{-18} g/cm^3 \quad \text{for} \quad t = 3 \cdot 10^7 years$$

The relative abundances $x(\mathrm{i})$ and $x^*(\mathrm{i})$ are calculated from a set of kinetic equations. The rates for the corresponding chemical reactions are calculated from data published in Woodall *et al.* (2007) and Aikawa *et al.* (1997). Table 1 contains the initial abundances. We have restricted our set of species to compounds having no more than seven atoms. In the ice phase only hydrogenation reactions are considered.

Table 1. Initial abundances of the elements in the gas phase, all other initial data are zero.

H	H_2	D	He	O	C^+	N	^{15}N	Si, Mg, Fe
0.9	0.1	1.5×10^{-5}	0.14	1.8×10^{-4}	7.3×10^{-5}	2.1×10^{-5}	1.1×10^{-7}	6.0×10^{-11}

From the calculated abundance evolution we obtain the time dependence of the ratios shown in Fig. 1. One recognises an increasing amount of non-polar ice and bounded heavy isotopes in the course of the prestellar core evolution. A large H_2 to H ratio seems to be advantageous for the formation of CO_2 relative to H_2O.

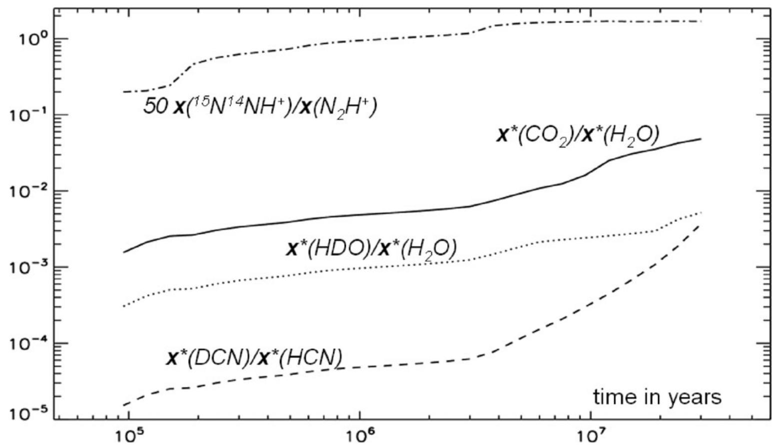

Figure 1. Time dependency of the nitrogen isotope ratio in the gas phase (note the factor of 50 to present all curves in the same figure), the D/H ratios in the ice phase and the CO_2-H_2O ratio for the polar to non-polar ice fraction calculated for the slowly evolving quasi-stationary prestellar core.

3. Simulation of the gravitationally collapsing protostellar cloud core

The gravitational collapse of a cloud core causes the central density to increase over more than 15-16 orders of magnitudes. At the end of this process a stellar core, the T

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Tauri star, and a young disk have formed in the centre of the solar nebula. Therefore, a numeric simulation of this type of collapse is a complex task. We have derived an analytical solution to solve the continuity, momentum and Poisson equation for a collapsing cloud core that is valid for spherical symmetry. According to Saigo *et al.* (2008) this restriction has no serious drawbacks as long as the rotation rate is low ($\approx 10^{-15}$ s^{-1}). The mathematics of this solution will be described in a different publication.

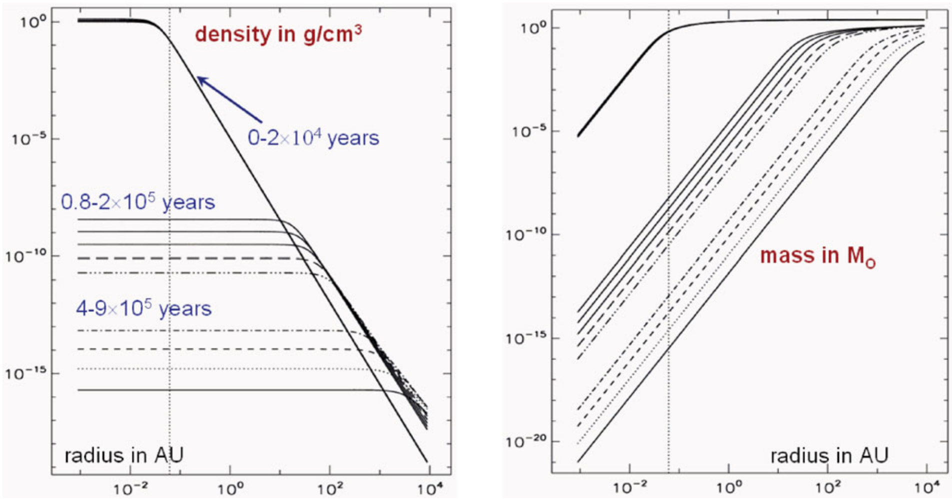

Figure 2. Density and mass profiles derived from the analytical model of the collapsing cloud core. The protostar is the so-called second core (Saigo *et al.* (2008)). The collapse takes place at the time t = 0.

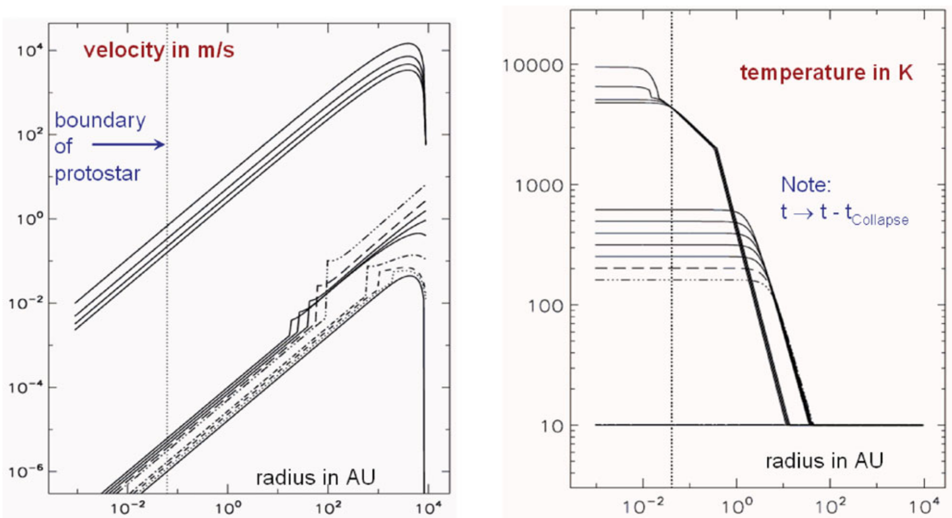

Figure 3. Velocity and temperature profiles derived from the same analytical model.

In Fig. 2 and Fig. 3 we present the calculated radial density, mass, velocity, and temperature profiles at different times. In order to include the influence of the formed protostellar disk we have coupled our collapse solution to the disk model derived by Stahler *et al.* (1994). The values of the four radial profiles in Fig. 2 and Fig. 3 are given for an Eulerian grid. However, the computation of the chemical abundance evolution of the gas and ice phase following from the continuity equation of each species can be simplified if one uses a transformation to a Lagrangian grid defined by the initial positions of the gas-ice parcels at the beginning of the collapse. The resulting total time dependencies of the density and temperature are calculated for an inner gas parcel moving from 2.5 to 1.3 AU. In this case the temperatures are high enough to guarantee the loss of the ice phase due to the evaporation of the icy grain mantles. In order to study the temporal progress of depletion of the ice phase species we have computed the ratio of the current to the initial abundance for selected compounds. The obtained values are presented in Fig. 4.

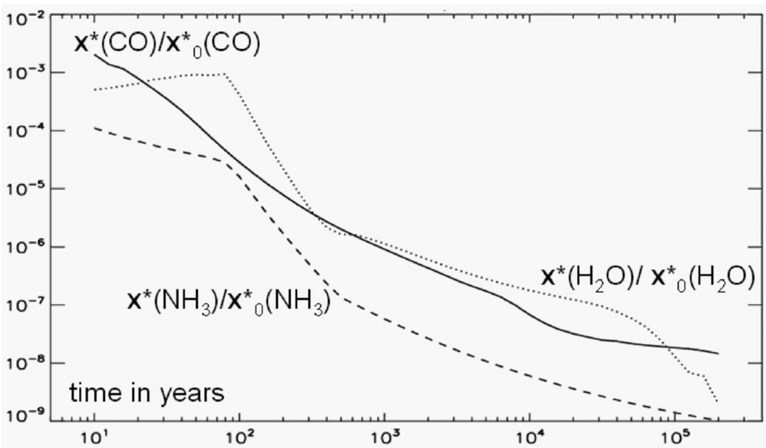

Figure 4. Time dependency of the ratio of the current to the initial abundance for CO, H_2O, and NH_3 calculated for the period of the collapsing protostellar core.

4. Simulation of the gravitationally collapsing protostellar cloud core

The disk model of Stahler *et al.*, 1994, is valid for a young disk only. In order to study the chemical evolution of the gas and ice species in a mature disk we have used the non-stationary model of Davis *et al.* (2003).

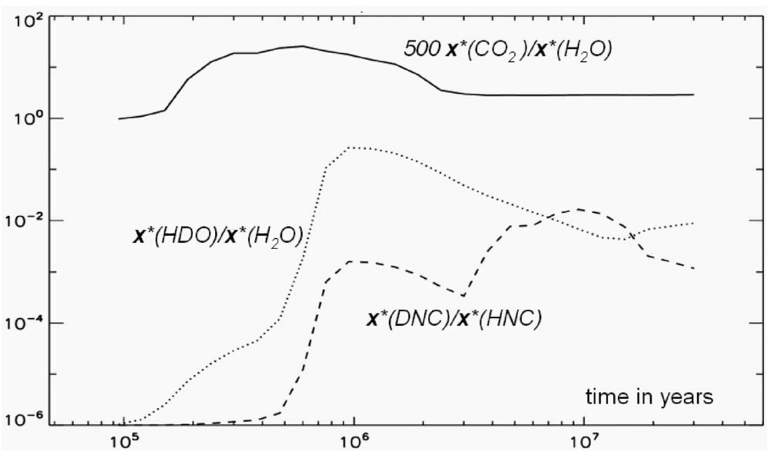

Figure 5. Time dependency of the D/H ratios in the ice phase and the CO_2-H_2O molecular ratio for the polar to non-polar ice fraction calculated for the evolving disk.

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This model describes the disk cooling and depletion in the course of its evolution. Due to the gas flow we have to switch to the Lagrangian grid again in order to compute the abundance values. The necessary initial data follow from the final abundance results calculated for the collapse period. In contrast to our collapse model the Davis model is based on axial symmetry. In order to keep a simple radial dependency without angular variations, the relative abundances are derived with respect to the column density. For time intervals much larger than 10^7 the corresponding number density would be less then $0.01\ \mathrm{cm}^{-3}$, i.e. a gas disk is not existent anymore. Therefore, at most 10 million years are of physical interest only. Fig. 5 shows the time behaviour of the same ice ratios as seen in Fig. 1. However, one recognizes clear differences although in both cases the ice phase abundancies are growing with respect of their initial values. For the evolving disk, there is a superposition of the time dynamics of the disk parameter itself and the time dynamics of the chemical processes. Therefore the shapes of the disk related abundance ratios versus time are less monotonic than the same curves of the prestellar core. In addition the disk density of the considered gas parcel decreases whereas the core density increases slowly.

5. Conclusion and outlook

The collapse of a rotating quasi-stationary cloud core into a young dense nebula and finally into a cooling disk is modelled in order to study the chemical evolution of the volatile gas and ice phase species. We have developed an analytical solution for the collapse period that gives the chance to simulate this process very efficiently. In addition we have studied the feasibility of merging the evolution periods of the solar nebula using the transition from an Eulerian to a Lagrangian grid. However, the transition from the spherically collapsing cloud core to the disk is complicated and further research needs to be done for the transition between the different temperature models. From our chemical calculations a distinct difference between the disk and the prestellar core chemistry becomes conspicuously. It is related to the higher dynamics in the disk on the one hand and to its complex initial chemical state on the other. The effects of both phenomenons are entangled and further research needs to be done to investigate their influence independently.

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