EPSC Abstracts
Vol. 8, EPSC2013-563, 2013
European Planetary Science Congress 2013

Evolution of the chemical composition in the solar nebula and its influence on the distribution of water

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Abstract

We have developed a multi-stage solar nebular (SN) model to investigate the water distribution from its earliest appearance in the parental molecular cloud (MC) to the planet forming disk stage. We estimate the radial distribution of different species ($H_2O, CO, HCN, NH_3, ...$) and the D/H ratio and test their sensitivity to different physical and chemical parameters like the radiation environment and the initial C/O ratio. We find that the D/H ratio in the cloud stage depends strongly on the utilized dust model and varies strongly in the region which constitutes the disk stage after collapse. Depending on the size of the hot corino, ice evaporation and warm gas-phase H_2O generation in the accretion region of the earth can be triggered. We evaluate how the D/H ratio change in the course of the SN evolution.

1. Introduction

Since the formation of water is a repetitive process, its deuterium to hydrogen D/H ratio depends on the physical conditions at different stages of the solar nebula. The earliest traces of water are found in the giant molecular clouds and their dark cores [2], which are the birthregions of stars. A consistent treatment of the chemical distribution in a solar system has thus to cover the complete history of chemical evolution. With this in mind we have constructed a SN model in which each of the three stages serves as the initial condition for the next. The three stages are oriented towards the temporal evolution of the SN, which can be separated into the following parts:

- a spherical core surrounded by the inter-core material of the parental cloud, which is in a critical hydrostatic equilibrium
- a collapsing core forming a protostellar source, an extending disk, and a spherical envelope, and
- an accreting geometrically thin disk in which gas and dust are moving with different velocities

The chemical code covers about 1900 species and includes dust surface chemistry and deuterium chemistry. It is based on the codes of Wakelam et al. 2006 [8] and Semenov & Wiebe 2011 [5], but expanded to include deuterisation. Each stage and the coresponding assumptions are summarized in the following Sec. 2, 3 and 4. We conclude the relevance to the water distribution in Sec. 5.

2. The Cloud Core

We start with a radial symmetric hydrostatic model of the core containing a gas-dust mixture in ISM concentrations with about one solar mass in total. The radial profile of gas and dust densities are evaluated in a self-consistent manner together with their respective temperatures. Both, gas and dust temperatures result from thermal balance equations and vary slightly with the dust distribution which changes due to the pressure of the interstellar radiation field.
We have validated our model by comparing the data of cloud core L134N [8] to the simulated abundance of a core with appropriate mass. For almost all chemical species sufficient agreement was found.

3. The collapsing core

Since the core is in a critical hydrostatic equilibrium, any small increase of the outer pressure causes its gravitational collapse. Therefore, we have simulated this collapse with a semi-analytical model based on a multi-zone density distribution. This model describes the formation of a central protostellar object surrounded by a viscous disk and a thin outer envelope.
A comparison of the radial profiles of the state variables given by Schönke & Tscharnuter 2011 [4] shows a good agreement except for the velocity which is

smaller in our model. We also compared the velocities with the radial profiles of Saigo et al. 2008 [3] and found an agreement in magnitude for radii > 10AU and slightly larger values in the inner region of their model. In conclusion, our velocity distribution suggests an outside - in collapse. Because the flux of material is much higher than in the hydrostatic cloud we model the chemistry in a Lagrangian frame.

4. The accreting Disk

The last period of the SN evolution, namely the disk stage, is modeled using a detailed dust convection model based on the stationary disk model of Takeuchi & Lin 2002 [7] to cover the optically thick phase of the disk. An important feature of this dynamical model is the differential treatment of gas and dust velocities, with the latter depending on the grain size. With the increase of solar radiation photoevaporation becomes important and the disk becomes optically and geometrically thin. We use a second disk model of Takeushi & Lin 2005 [6] to account for these processes. To derive the temperatures in both optical regimes (thick and thin) we use the radiation hydrodynamics code of Bitsch et al. 2013 [1] in the flux limited diffusion limit. As in the previous stage the chemistry is treated in a Lagrangian approach in which non-interacting volumes of matter propagate along the velocity field and undergo reactions depending on the local conditions.

5. Summary and Conclusions

According to our simulations, the relative water abundance in the core depends on the temperature profiles of gas and dust, the UV radiation of the ISRF and the initial element ratios, especially metallicity and C/O ratio. The interaction between dust and radiation influences the total amount of water in the core only marginally with time, but the radial profiles vary clearly. The dust contains 10^{6-7} times more water as the gas phase, because of the low formation efficiency of H_2O in cold gas ($\sim 10K$). Roughly 35.7% of the oxygen atoms are incorporated into water molecules, if the intensity of the ISRF is about 1 Habing. This number increases to 38.5% if this intensity triples. The D/H ratio shows the stongest radial gradient in the region between $5-6$ kAU where it varies about one order of magnitude. Because most of the non-deuterized water is stored as ice in the outer regions, the total water concentration has its highest amount there. (See. Fig. 1)

The obtained inner water amount of the collapse is

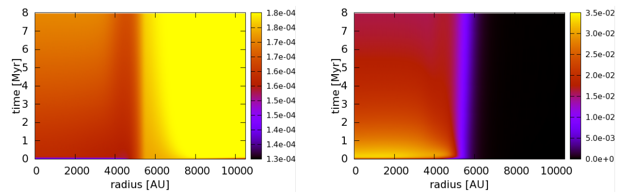

Figure 1: left: total water concentration in the core, right: D/H - ratio in the water fraction

similar in magnitude to the data reported in literature (Aikawa et al. 2008; Visser et al. 2009, 2011) but our abundance profiles vary stronger with the radius. We compare the D/H ratio of the water directly formed in the gas phase or being desorbed into the gas from the dust grains with the D/H values observed for comets. We further investigate how radial mixing in the disk stage can alter the radial gradient in the D/H ratio.

Acknowledgements

This work was supported partly by the Helmholtz Alliance on “Planetary Evolution and Life”. We are very grateful to Valentine Wakelam, Dmitry Semenov and Bertram Bitsch for providing their codes to us.

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