

# Chemical changes during transport from cloud to disk

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**Abstract.** We present the first semi-analytical model that follows the chemical evolution during the collapse of a molecular cloud and the formation of a low-mass star and the surrounding disk. It computes infall trajectories from any starting point in the cloud and it includes a full time-dependent treatment of the temperature structure. We focus here on the freeze-out and desorption of CO and H<sub>2</sub>O. Both species deplete towards the centre before the collapse begins. CO evaporates during the infall phase and re-adsorbs when it enters the disk. H<sub>2</sub>O remains in the solid phase everywhere, except within a few AU of the star. Material that ends up in the planet- and comet-forming zones is predicted to spend enough time in a warm zone during the collapse to form complex organic species.

**Keywords.** Planetary systems: protoplanetary disks, circumstellar matter, stars: formation, astrochemistry

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## 1. Introduction

The chemical composition of the building blocks of planets and comets depends on the chemical evolution throughout the formation process of a low-mass star and its circumstellar disk, where the planetary and cometary building blocks are to be found. The chemistry in pre-stellar cores—essentially molecular clouds that will collapse to form a star at some point—is relatively easy to model, because the dynamics and the temperature structure are simpler before the protostar is formed than afterwards. A key result from the pre-stellar core models [see Lee *et al.* (2004) for a short review] is the depletion of many carbon-bearing species towards the centre of the core.

Ceccarelli *et al.* (1996) were the first to model the chemistry in the collapse phase, and others have done so more recently (e.g. Rodgers & Charnley 2003, Lee *et al.* 2004, Aikawa *et al.* 2008). All of these models are one-dimensional, which necessarily leaves out the circumstellar disk. As the protostar turns on and heats up the surrounding material, all models agree that frozen-out species return to the gas phase if the dust temperature surpasses their evaporation temperature. The higher temperatures can further drive a hot-core-like chemistry, and complex molecules may be formed if the infall timescales are long enough.

If the disk is included, the system gains a large reservoir where infalling material from the cloud can be stored for a long time before accreting onto the star. The inner parts of the disk are shielded from direct irradiation by the star, so they are colder than the

disk's surface and the remnant cloud. Hence, molecules that evaporated as they fell in towards the star may freeze out again when they enter the disk.

We present here the first semi-analytical model that follows the chemical evolution from the pre-stellar core to the disk phase in two dimensions. We trace individual parcels of material as they fall in from the cloud into the disk, and we analyze the gas/ice ratios of CO and H<sub>2</sub>O in these parcels. This gives us a first indication of what happens to complex organics during the infall process. Finally, we briefly discuss the model results in light of the chemical diversity found in comets.

## 2. Description of the model

Our model solves the chemistry in a two-dimensional axisymmetric Lagrangian frame. It takes a parcel of material at some starting point in the cloud and uses time-dependent velocity fields to follow it into the star or disk. The density and temperature are computed at each point. Photoprocesses are ignored, except that stellar photons are used as a heating source. A full description of the model will appear in an upcoming paper (Visser *et al.*, in prep.); only the main features are summarized here.

The densities and velocities in the cloud are taken from Terebey *et al.* (1984), who added rotation to the well-known inside-out Shu (1977) collapse. The model switches to the Cassen & Moosman (1981) solution inside the centrifugal radius,  $R_c$ . The infall trajectories are radial at large radii and deflect towards the midplane closer in; they finally intersect the midplane inside of  $R_c$ . This causes a build-up of material in a thin layer around the star: the circumstellar disk. Conservation of angular momentum causes part of the disk to spread out beyond  $R_c$ . As soon as this happens, accretion from the cloud onto the extended part of the disk is also allowed. The radial dynamics of the disk are treated as in Dullemond *et al.* (2006). The vertical density profile is taken to be a Gaussian at all times and the vertical velocities are chosen such as to accomplish this. The dust temperature in the entire system is calculated with full radiative transfer (Dullemond & Dominik 2004) and the gas temperature is assumed to be equal to the dust temperature everywhere. Shocks were found not to be important beyond 0.1 AU for material entering the disk more than  $3 \times 10^4$  yr after the onset of collapse (Neufeld & Hollenbach 1994). A bipolar outflow, perpendicular to the disk, arises naturally from the Terebey *et al.* (1984) solution and is included as an evacuated cavity.

At first, the only chemistry included in the model is the adsorption and desorption (freeze-out and evaporation) of carbon monoxide (CO) and water (H<sub>2</sub>O). Their overall abundance remains constant throughout the collapse. The reaction rates are from Rodgers & Charnley (2003), except for the H<sub>2</sub>O desorption, which is from Fraser *et al.* (2001). A network including chemistry beyond adsorption and desorption will be included in the future. CO and H<sub>2</sub>O begin fully in the gas phase and a  $10^5$ -yr static pre-stellar core phase is included before the onset of collapse.

In our standard model, all CO evaporates at a single temperature. In reality, however, CO is mixed with the H<sub>2</sub>O ice, and some of it will be trapped until the H<sub>2</sub>O desorbs (Collings *et al.* 2004). This effect can be approximated by letting part of the CO evaporate at higher temperatures. Specifically, a scheme with four “flavours” of CO ice was used (Viti *et al.* 2004) as an alternative to the standard model.

Some organic species, e. g. methanol (CH<sub>3</sub>OH), are likely to be formed in the pre-stellar core (Garrod & Herbst 2006). Other organics, primarily the more complex ones like methyl formate (HCOOCH<sub>3</sub>), are only formed if an infalling parcel spends at least several  $10^4$  yr in a warm, 20–60 K, region. The binding energy of both classes of organics is similar to or higher than that of H<sub>2</sub>O, so they desorb at the same or at higher temperatures.

Freeze-out occurs at about the same rate as for  $\text{H}_2\text{O}$ . Hence, the  $\text{H}_2\text{O}$  gas/ice ratio is an upper limit to the organics gas/ice ratio.

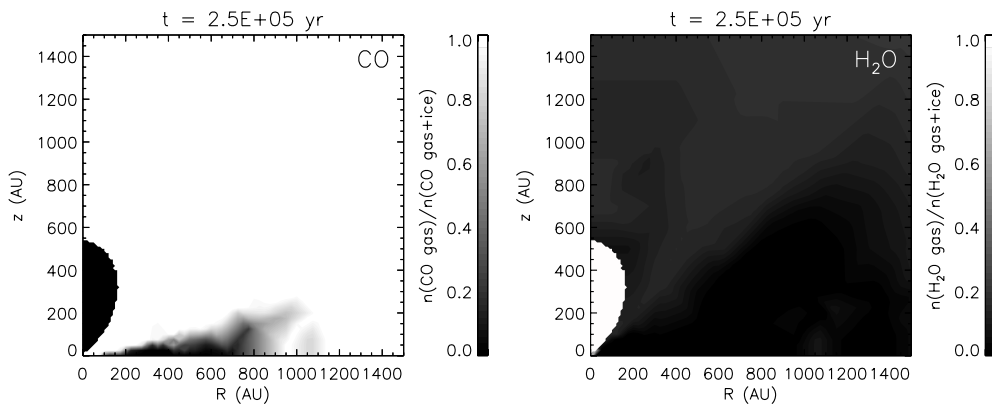
### 3. Results

Results are presented here for our standard model with an initial cloud mass of  $1.0 M_\odot$ , a cloud radius of 6700 AU, an effective sound speed of  $0.26 \text{ km s}^{-1}$ , a solid-body rotation rate of  $10^{-13} \text{ s}^{-1}$ , and an initial uniform temperature of 10 K. After the onset of collapse, the outer parts of the cloud reach the disk in  $2.5 \times 10^5 \text{ yr}$ . The centrifugal radius at that time is 500 AU and the disk has spread to about 700 AU.

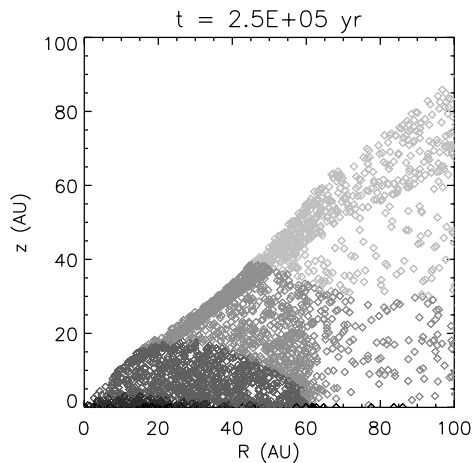
During the  $10^5$ -yr pre-stellar core phase, CO and  $\text{H}_2\text{O}$  freeze out inside of  $\sim 4000 \text{ AU}$  and remain in the gas phase further out. This is consistent with other pre-stellar core models. The disk becomes important and the system loses its spherical symmetry at  $t \approx 2 \times 10^4 \text{ yr}$ . Up to that point, our results are the same as those from the 1D models. The collapsing region quickly heats up to a few tens of K, driving CO (evaporating around 20 K in the one-flavour model) into the gas phase, but keeping  $\text{H}_2\text{O}$  (evaporating around 100 K) on the grains.

After  $\sim 2 \times 10^5 \text{ yr}$ , the disk has become massive enough that the temperature drops below 20 K near the midplane. CO arriving in this region re-adsorbs onto the grains and another  $5 \times 10^4 \text{ yr}$  later, there is a significant amount of solid CO in the disk (Figure 1). Some solid CO also exists in the remnant cloud just beyond the disk, which is shielded from direct irradiation. Outside of 1000 AU, the cloud is thin enough that scattering from higher altitudes causes a slightly higher temperature ( $\sim 25 \text{ K}$ ), keeping most CO in the gas phase. The border between the solid and gaseous CO regions lies close to the 20-K surface, showing that the re-adsorption is a fast process.  $\text{H}_2\text{O}$  is still predominantly frozen out at this time, but there can be up to 20% in the gas phase in the warmer regions above the disk. Within a few AU from the star, all  $\text{H}_2\text{O}$  has evaporated.

In the model with four flavours of CO ice, 13% of the CO desorbs at 70 K and 6.5% desorbs at 100 K (Viti *et al.* 2004). This has the expected effect of keeping about a fifth of the total CO in the solid phase throughout the fully gaseous region of the one-flavour model. The region with at least 80% of solid CO extends to the same radius in the



**Figure 1.** Fraction of gaseous CO (left) and  $\text{H}_2\text{O}$  (right) in the disk and remnant cloud  $2.5 \times 10^5 \text{ yr}$  after the onset of collapse. The outflow region, extending out to 540 AU in the vertical direction, is indicated in black on the CO plot and in white on the  $\text{H}_2\text{O}$  plot. The one-flavour model was used for the CO desorption.



**Figure 2.** Locations of a number of parcels in the disk  $2.5 \times 10^5$  yr after the onset of collapse. The lighter a parcel, the later it entered the disk, and the further out in the cloud it originated.

four-flavour model as in the one-flavour model, and is about twice as large vertically. This corresponds to a total solid CO mass in the disk that is approximately 50% higher.

The disk roughly maintains a layered structure throughout the accretion phase, because new material is always deposited on top (Figure 2). Material near the midplane at  $t = 2.5 \times 10^5$  yr typically accreted close to the star and moved out to its current position due to conservation of angular momentum. This material spent several  $10^4$  yr at 20–60 K during that process, sufficient for the formation of complex organic species (Garrod & Herbst 2006). Smaller organic species will have formed already in the pre-stellar core. Taken together, our model predicts that organic species are abundant in the planetary and cometary building blocks for our standard set of parameters. All the organics are expected to be in the solid phase in the disk outwards of 5–10 AU at  $t = 2.5 \times 10^5$  yr, along with  $\text{H}_2\text{O}$ . A full chemical network needs to be run to quantify the organic abundances in the building blocks. An interesting test case, to be analyzed in a future paper, is the chemical diversity found in comets (Bockelée-Morvan *et al.* 2004, Mumma 2008). If a similar range of abundances is found in our model at different radii, this might explain some of the cometary abundances.

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## Discussion

MUMMA: About the last point, are you talking here about pure CO ice as opposed to the mixed water ice?

VISSER: If you use pure CO ice, then almost all will evaporate first and then freeze out in the disk. If you take the mixed CO ice, then part of the CO will remain frozen, mixing with water.

HENNING: The result must depend on the initial angular momentum assumed for the molecular cloud because that defines where the material ends up in the disk?

VISSER: We are using a model with a very high rotation rate of  $10^{-13} \text{ s}^{-1}$ . We plan to do a parameter study and the rotation rate is one of the things that we will be modifying. As you say, it may have a large influence on the result here.

SANDFORD: I would be a little cautious about the statement associated with formaldehyde, when Willem Schutte was in our lab many years ago, he demonstrated that when you have  $\text{H}_2\text{CO}$  in your ice and you warm up, and it can very easily polymerize into different components depending on what other molecules are in the ice. Even if there's just slightest trace of ammonia in the ice the polymerization can be very efficient. So it's quite possible that the  $\text{H}_2\text{CO}$  won't act as inert as the model seems to imply.

VISSER: Clearly we need to go to a complete chemical network if we want to really understand it in details. We just took formaldehyde as a random species mostly with a binding energy between oxygen and water just to see what we can get in terms of the gas in the ice.



Kasandra O'Malia (photo by Dale Cruikshank).