Reliability of the disk chemical modeling

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Summary

Using analysis of uncertainties in the reaction rates coefficients of a gas-grain chemical model of low-mass TTau protoplanetary disk, we identify the observable molecules which model abundances are not greatly influenced by the rate uncertainties. We also demonstrate that the rate coefficients of only a handful of chemical reactions need to be determined more accurately in order to improve the reliability of disk astrochemical models.

Model

We utilized the 1+1D steady-state model of a typical low-mass protoplanetary disk of DM Tau [1] that have M_{disk} = 0.03*M*sun, and *R*disk = 800 AU. A gas-phase chemical model with accretion and desorption processes based on the RATE'06 [2] database was applied. The reaction rates were randomly varied within their uncertainty limits 8000 times. We adopted the "low metals" initial concentrations and allowed chemistry to evolve over 5 Myr.

1. How large the abundance scatters for observationally important species?

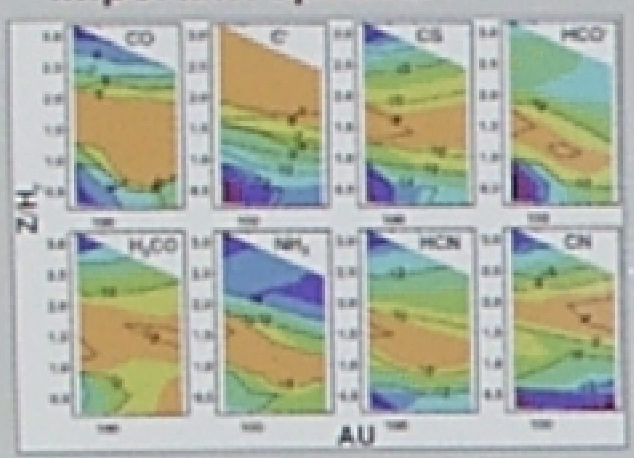

Figure 1. Averaged molecular abundances at 5 Myr.

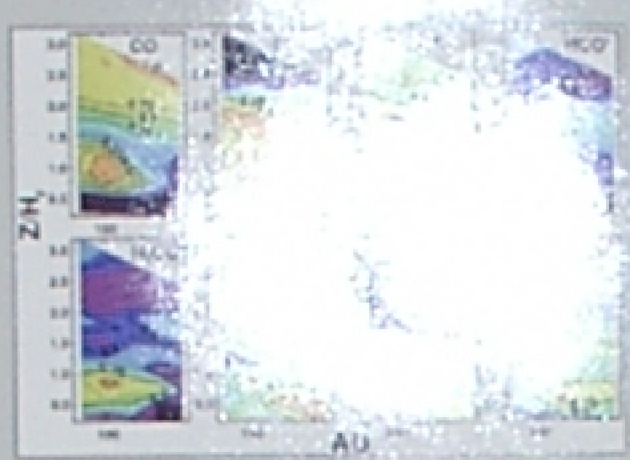

Figure 2. Dispersions of abundances at 5 Myr.

The relative averaged abundances of observable molecules vary greatly through the disk (Fig.1), though the overall distribution still resemble layered "sandwich"-like structure. While it appears rather smooth, the abundance dispersions may be large even for simple molecules in some disk regions due to rate uncertainties (Fig.2).

The computed abundance dispersions at 5 Myr differ substantially through the disk, but in general do not exceed a factor of 3—4 even for complex species. Note that there is a disk region with high dispersion for almost every carbon-bearing species in the intermediate layer (R=100AU, Z/H=1.0,Fig. 2).

2. Which reactions define the resulting abundance scatters to the largest extent?

We apply a modified version of statistical correlation method described in [3,4] to discriminate the gas-phase chemical reactions that cause the largest uncertainties in the calculations. Though this technique was applied for individual disk points, the results were summed up to get the global trends. Using this scheme, we designate most "uncertain" chemical reactions that cause the largest uncertainties in the abundances of species in the entire disk (see Table below).

H_2	+	C	=	CH_2	+	*hv*
C^+	+	H_2	=	CH_2^+	+	*hv*
C	+	*hv*	=	C^+	+	e^-
H_2	+	c.r.p.	=	H_2^+	+	e^-
He	+	c.r.p.	=	He^+	+	e^-
N	+	c.r.p.	=	N^+	+	e^-
N	+	CH_2	=	HCN	+	H
H_2	+	CH_3^+	=	CH_5^+	+	*hv*
C	+	crphot	=	C^+	+	e^-
CH_2	+	S	=	CS	+	H_2

Table 1. "Most uncertain" reactions in the disk at 5 Myr.

3. Which species might be used as "uncertainty-independent" molecular tracers?

In order to estimate how large will be the abundance and column density scatters when the most important rates will be obtained more accurately, we decrease the rate uncertainties of the 57 most important reactions to factors of 1.25—2. These 57 reactions represent only 1% of the total amount of reactions in the chemical model.

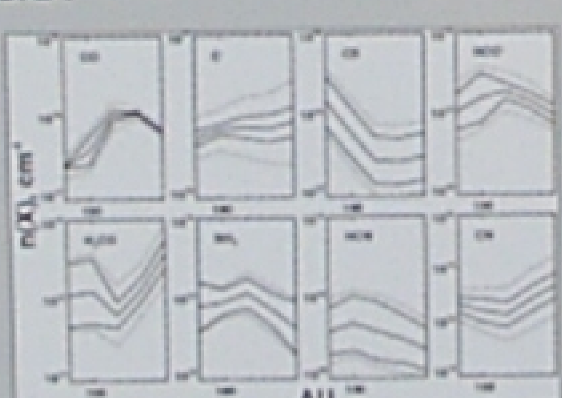

Figure 3. Scatters in modeled column densities at 5 Myr.

In Fig. 3 the column densities with error bars are shown for the standard RATE06 model (dotted line) and for the model where the 57 important reactions have small rate uncertainties (solid line). As can be clearly seen, dispersions of the column densities are not greater than a factor of 3 even for the standard model, which is comparable with the accuracy of observational data. With the improved rates of only 1% of the RATE06 reactions, the column density uncertainties decrease, especially for C^+ and CN.

1. Hypersensitivity in the disk

In Fig. 4 shapes of abundance distributions are shown. In most disk points it is a Gaussian (bottom panel), but in one point near R=100AU, Z/H=1.0 this shape is more complex and shows two-peak behavior.

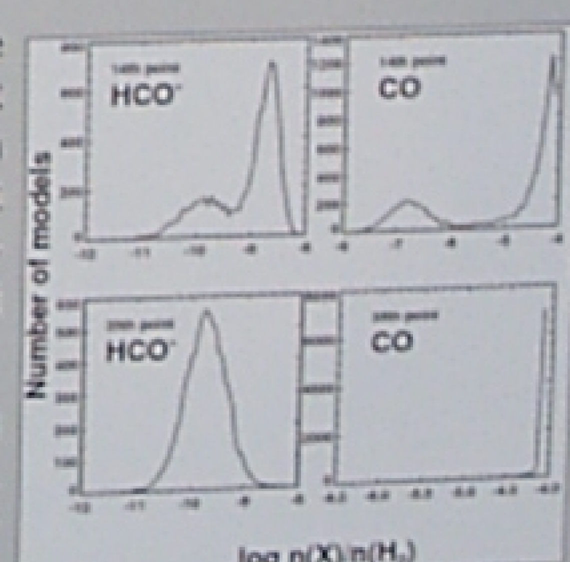

Figure 4. Shape of abundance distributions of HCO^+ and CS in hypersensitivity (top) and normal (bottom) points of the disk.

In this region the so-called hypersensitivity of abundances to the rate constant of the X-ray ionization of He appears [4]. He ions are able to dissociate CO and produce C^+ at late times of $>10^5$ years, which is used to build up carbon chains and cyanopolyynes that are immediately frozen out onto grain surfaces.

In turn, it leads to the complex behavior of other carbon-bearing species and results in a complex shape of the corresponding abundance distributions (top panel). Deviation from Gaussian shape is the main reason of the large dispersions in this disk region.

References

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