Non-stationary chemistry in protoplanetary disks

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Introduction

Transport phenomena constitute an inherent factor of protoplanetary disk evolution. There are many observational facts indicative of the compositional large-scale radial mixing, e.g, the presence of the crystalline dust in comets and protoplanetary disks, anomalous isotopic abundances in meteorites and distribution of water ice in the Solar Nebula (e.g., Boss 2004; Wooden et al 2005).

However, in the astrochemical community the disk evolution is often considered from the purely chemical point of view, so that a disk is treated as having no internal motions or having only inward advection (e.g., Aikawa & Herbst 1999). By now, there are only two published works where the diffusive transport in protoplanetary disks is treated in conjunction with the time-dependent chemistry. Ilgner et al. (2004) have considered vertical diffusion and radial advection in the inner part of a protoplanetary disk (in the 1+1D approximation) to study the effect of mixing on the sulfur chemistry. In Ilgner & Nelson (2006) the influence of the vertical diffusive transport is studied in relation to the fractional ionization in the inner part of a protoplanetary disk.

In this presentation, we study the influence of a turbulent (non-static) chemical processes on the disk chemical evolution and argue that in order to assess the importance of diffusive transport processes one has to consider vertical and radial mixing simultaneously.

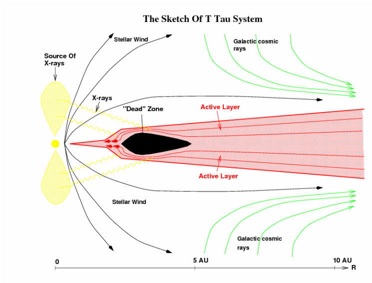

FIG.1: Sketch of a young T Tau system consisting of a star surrounded by a disk of gas and dust. Non-thermal stellar UV and X-ray radiation as well as interstellar UV photons and cosmic rays are the main ionizing sources. Chemically, disk can be divided on three distinct zones: 1) dark, cold midplane where molecules mosly freeze out onto grains, 2) warm, chemically rich intermediate layer where line emission comes from, and 3) surface layer of simple atomic and ionic composition.

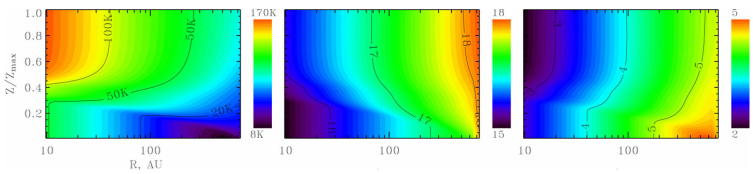

FIG.2: (From left to the right) The disk temperature structure (K), the diffusion coefficient ($cm^2\,s^{-1}$; log scale), and the characteristic mixing timescale (years; log scale) in the DM Tau disk. The Y-axis represents the normalized vertical height, $z_0(r) = z(r)/z_{max}(r)$.

Modeling

We use a steady-state disk model of DM Tau (see D'Alessio et al. 1999). The disk has a radius of 800 AU, an accretion rate $M_{dot} = 10^{-8} M_{sun}\,yr^{-1}$, viscosity parameter $\alpha = 0.01$, and a mass of $0.03 M_{sun}$. We focus on outer disk part, R>10 AU (see Figs. 1, 2). The diffusion coefficient is computed as $K = \alpha\, c_s\, h$, where c_s is sound speed and h is the local scale height, and its typical values in disks are about 10^{16} — 10^{18} $cm^2\,s^{-1}$ (Fig.2, middle panel). Consequently, characteristic mixing timescale can be estimated as $t=h^2/K$ (Fig.2, right panel).

Applying the reduction techniques described in Wiebe et al. (2003), we isolated the gas-grain UMIST'95 network with surface reactions consisting of 263 species and 1200 reactions, which allows to follow the evolution of key molecules (CO, HCN, H_2O, H_2CO, DCO^+, HDO, and some others) with reasonable accuracy. The equations of the chemical kinetics are solved simultaneously with the diffusion terms in the Eulerian description, using a fully implicit 2D integration scheme. All the equations are solved on a non-uniform staggered grid consisting of 30 radial points and 65 vertical points. This resolution was found to be optimal for mixing problems in a protoplanetary disk. The evolutionary time span is 5 Myr.

Our simulations consist of five runs. The first run represent the stationary chemical model in which no transport processes are taken into account. In the second run vertical mixing is added. In the third run, the stationary chemistry is modeled. Both vertical and radial mixing is accounted for in the fourth run. Fifth run is the same as fourth model but with the 100 times lower diffusion (see Fig. 3).

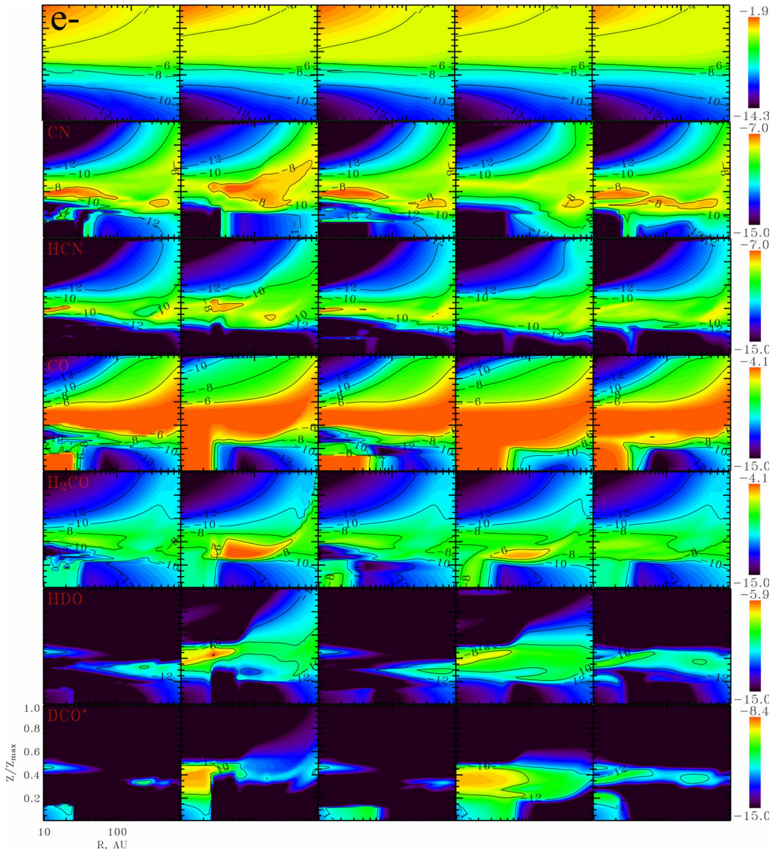

FIG.3: (From left to the right) Molecular abundances in DM Tau disk at 5 Myr computed with 5 different gas-grain chemical models: 1) stationary chemistry, 2) chemistry with mixing in vertical direction, 3) chemistry with mixing in radial direction, 4) chemistry with mixing in radial and vertical directions, and 5) the same as 4) but for 100 times lower diffusion coefficient. Shown are relative gas-phase concentrations of e^-, CN, HCN, CO, H_2CO, HDO, and DCO^+ (in respect to the amount of hydrogen nuclei).

Results

1) Diffusion affects the disk abundances and column densities of some molecules, but not all of them. The most notable exception is the ionization fraction that is not sensitive to the mixing . This holds true for many other simple species produced by photochemistry, e.g., C_2H, CN, and HCN (see Fig. 3).

2) Turbulent mixing allows to sustain a large reservoir of the CO gas in the coldest disk parts, where T<20 K and where thus freeze out proceeds very fast – a feature that cannot be explained in framework of the static chemical models. Such abundant, exremely cold CO gas has indeed been detected in the DM Tau disk by Dartois et al. (2003).

3) Transport processes may lead to significant enhancement of the gas-phase H_2CO concentration through the entire disk, up to a few orders of magnitude. Moreover, this enhancement depends strongly on the adopted diffusion efficiency, so thus this molecule may serve as an observable tracer of the degree of the disk turbulence. The main reason is that the evolution of this complex organic species is governed by surface reactions, which proceed more slowly than dynamical processes, $t_{chem} > t_{mix}$.

4) Mixing also tends to increase mixing-dependently the gas-phase abundance of deuterated molecules, like HDO and DCO^+.

5) Note that one has to consider a combination of radial and vertical mixing components simultaneously in order to get feasible results.

References

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