CEPD – Chemical Evolution of Protoplanetary Disks

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Abstract

Protoplanetary disks undergo a significant evolution from their early phase of a hot, protostellar core towards a debris disk. We present a new project on the physical and chemical evolution of protoplanetary disks in their intermediate phase. Thereby, we plan to focus especially on the effects of turbulent mixing on the chemical composition in the disk. Strong turbulence might drive the disk's chemistry out of equilibrium and replenish the abundances of molecules in the inner disk and the upper layers, where they are continuously destroyed by incident X-ray radiation.

To address the complex problem of modeling the combined evolution of the disks' physical and chemical state and to confront it with observations, we propose a step-by-step approach. Here, we demonstrate the molecular line emission of the inner regions of protoplanetary disks. The disk taken to be static and based on an extended, irradiated α-viscosity disk model, while the chemical abundances are calculated as a function of time over 10^7 years. Our first results on radiative transfer analysis suggests that molecules such as H_2O, CO and CH_4 indeed can be detected in the inner 20AU of the disk, although further studies are needed for a firm proof of our results.

Introduction

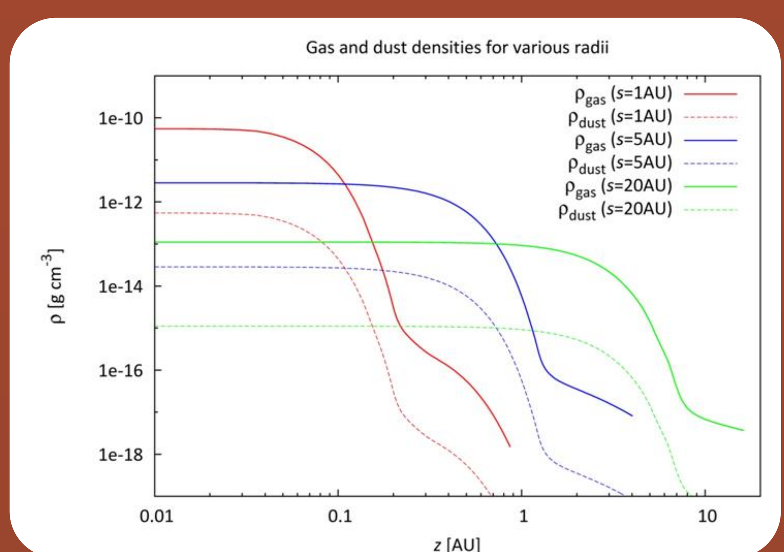
Protoplanetary disks are considered as a natural environment for the creation of simple and complex molecules which may ultimately lead to the evolution of life. Recent observations of the young protoplanetary disk of AA Tauri reveal a basic, active organic chemistry and important molecules such as H_2O, OH, CO_2 and CO being abundant within the inner disk (Carr & Najita, 2008). Naturally, observations probe the chemical composition close to the disk surface in the optically thick disk, where continuous photodissociation by stellar, interstellar and cosmic radiation should lead to a depletion of these molecules. A steady supply of the inner disk region with these elements implies that the disk sustains an active accretion of material from further outwards, where these molecules are frozen onto dust grains.

Such a scenario has been proposed and studied recently (e.g., Nomura et al., 2008). In this work, we studied the implications of an ongoing, strong accretion in protoplanetary disks on the observation of molecular emission lines. We calculated the methanol emission from the inner disk region in the simple case of a disk seen face-on. For the case of methanol, we confirm the observational indications of increased abundances in the inner disk. To provide a better ground for these conclusions, we extend the model by studying the abundances of commonly observed molecules in the inner disk .

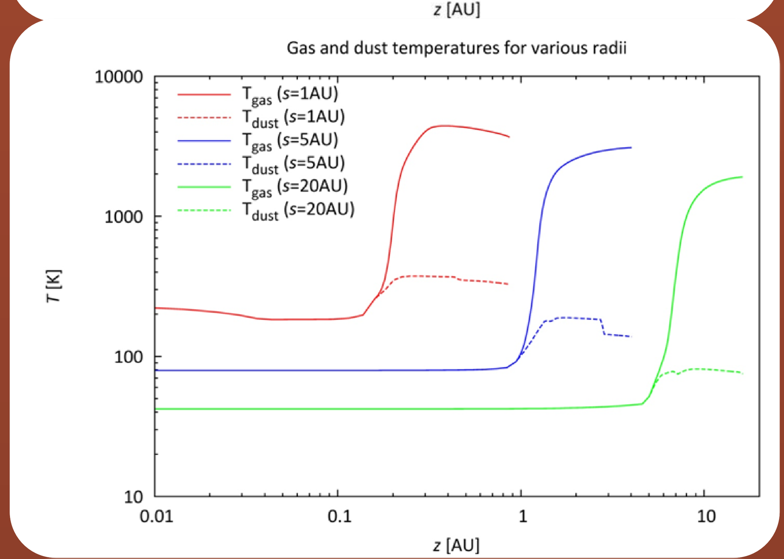
Underlying protoplanetary disk model

The underlying disk model is taken from Nomura et al. (2007), who calculate an axisymmetric disk around a typical T Tauri star (with M=0.5M_{sol}, R=2R_{sol}, T=4000K).

In this model, the gas temperature and density are calculated under the assumption of hydrostatic equilibrium in the vertical direction and local thermal balance between heating and cooling. Grain photoelectric heating by far ultraviolet photons, X-ray heating by hydrogen ionization, gas-grain collisions and radiative cooling by line transitions are incorporated in the model.

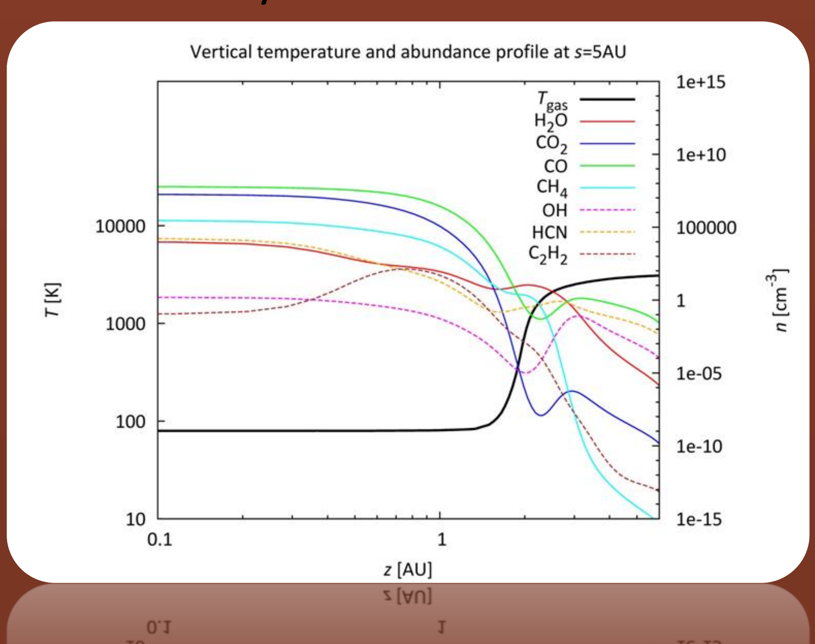


The dust temperature is derived self-consistently by solving the 2D radiative transfer equation (c.f., Dullemond & Turolla 2000, Nomura 2002). It is assumed that gas and dust are well mixed with a constant dust-to-gas ratio 0.01 in the disk. Typical temperature and density distributions in the vertical direction are displayed here for radii s={1,5,20}AU.



Chemical reaction network

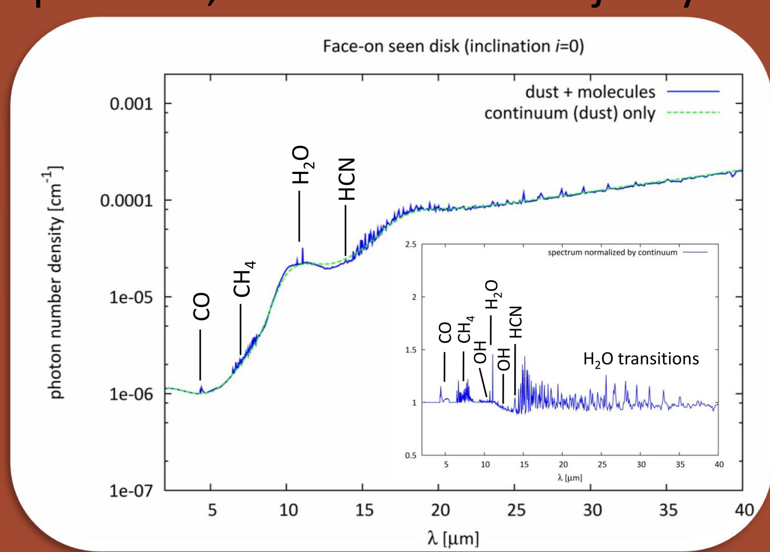
We use the UMIST Database for Astrochemistry (Millar et al., 1997) to calculate the chemical reactions in the disk for 10^7 years. We apply the DVODE package (Brown et al., 1989) to solve the set of differential equations for 209 species which are connected by 2960 reactions. We also account for photodissociation of the molecules in the upper, low-density layers of the disk by incident cosmic radiation with a simple model. We do not consider for the depletion of molecules onto dust grains in the colder disk midplane. Also, the effects of dynamical motion, such as accretion flows and turbulent mixing, are not included here.



Typical abundances of the species of most interest are displayed here as a function of distance from the disk plane at s=5AU.

Molecular emission line spectra

We adopt a parallel line-of-sight integration to calculate the emerging spectra from the underlying disk in the near- and mid-infrared. Thereby, the bulk continuum flux is provided by the star and the dust, with the star assumed as blackbody emitter with T=4000K. Dust absorption and emission is taken from the Jena dust-opacity tables (Ossenkopf & Henning, 1994). Species of most interest are, due to the availability of observational data, H_2O, CO_2, CO, CH_4, OH, HCN, and C_2H_2. Energy levels and line transitions are taken from the HITRAN database (Rothmana et al., 2005). We calculate emission spectra from the inner disk region, s=1-20AU, in the wavelength range of 2-40µm. Here, we show first results of the spectra for the case of a face-on disk. A number of prominent molecular emission lines can be detected in the spectrum, with the vast majority of the lines being due to the rotational transitions of H_2O. We are able to detect molecular line emission from all molecules except C_2H_2, which stands in contrast to observational data (c.f., Carr & Najita, 2008). Interestingly, recent theoretical work (Woods et al., 2008) claims that C_2H_2 is strongly affected by photodissociation and therefore not abundant in the hotter layers where line emission occurs. A careful treatment of the photodissociation process, in combination with chemical reactions that may efficiently produce C_2H_2 (Agúndez et al., 2008), and/or a further supply of C_2H_2 by dynamical motion inside the disk is required to clarify the observed abundances at the disk surface.



Roadmap towards CPEPD

Efficient accretion requires strong turbulence in the disk, which, through turbulent mixing, may drive the chemical composition out of equilibrium. Radial turbulent mixing may increase the abundance of the observed molecules in the inner disk region, while the effect of vertical turbulent mixing strongly depends on the timescales involved: if vertical mixing is able to transport molecules from the disk midplane into the upper layers faster then they are dissociated, we expect stronger molecular line emission. The main purpose of our future work therefore is the investigation of the effects of turbulence in protoplanetary disks by modeling the radial *and* vertical turbulent mixing and calculating the emerging molecular line emission from these systems. Ultimately, a time-dependent modeling of the physical *and* chemical evolution of the disk, including turbulent mixing, together with a continuous radiative transfer analysis, will enable us to predict the evolution of protoplanetary disks from theory and to confront it with latest observations.

A self-consistent model needs to relate the description of the turbulence to the viscosity in the disk. Today, it is widely believed that magnetic effects are the main contributor through the magneto-rotational instability (Balbus & Hawley, 1991). Despite its success, the MRI suffers from the fact that ionized material is necessary to couple to the magnetic field – dead zones occur otherwise. As pointed out recently (Heinzeller, 2008), convective heat transport can also give rise to considerable turbulence, which, in the case of low-temperature protoplanetary disks, requires shadowing of the stellar radiation to create the necessary temperature gradients. The dead zones thus might be enlivened by turbulent transport of ions into these regions, caused by convection and the MRI itself (Ilgner & Nelson, 2008).

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