CEPD — Chemical Evolution of Protoplanetary Disks

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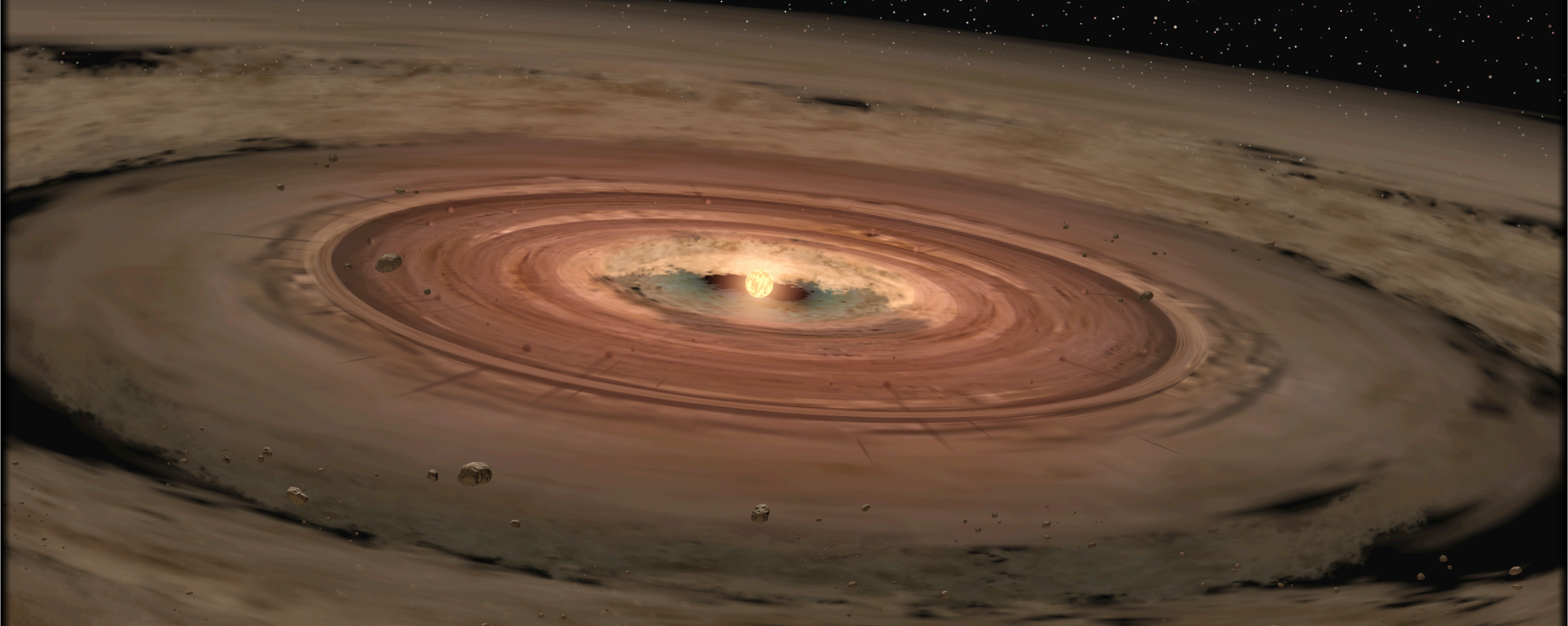
Protoplanetary disks undergo a significant evolution from their early phase around a hot, protostellar core to their dispersal phase after planet formation. As such, they represent a natural and active environment for the creation of simple and complex molecules which may ultimately lead to the evolution of life.

Recent observations of protoplanetary disks around T Tauri stars reveal an active organic chemistry and important molecules such as H_2O, OH, CO_2 and CO being abundant in the inner disk (e.g., Carr & Najita 2008, Salyk et al. 2008). Observations probe the chemical composition close to the disk surface in the optically thick disk, where these molecules are photodissociated continuously by stellar, interstellar and cosmic radiation. A steady supply of the inner disk with these elements might be required to account for the observations.

We present a new project on the chemical evolution of protoplanetary disks in their intermediate phase. Thereby, we plan to focus especially on the effects of turbulent mixing and accretion motion on the chemical composition: strong turbulence might drive the disk chemistry out of equilibrium and replenish the abundances of molecules in the inner disk regions and in the upper disk layers. Likewise, inward accretion may supply the inner disk with molecules from the outer regions where they are frozen onto dust grains.

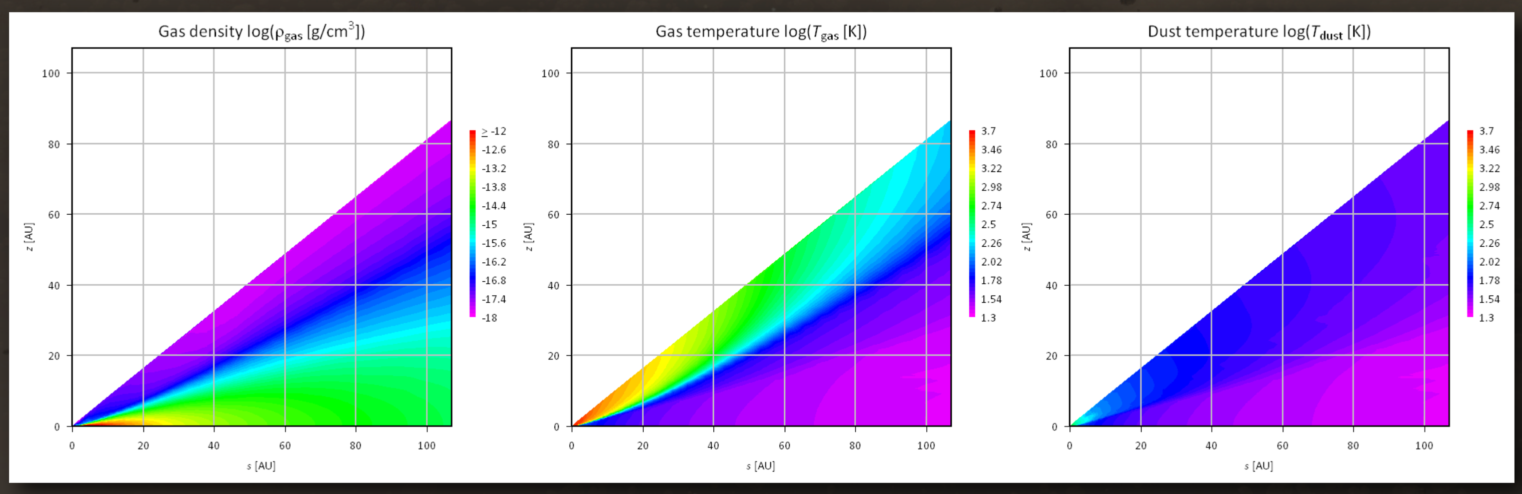
We address the problem of modeling the combined evolution of the disks' physical and chemical state in a step-by-step approach. Here, we calculate the molecular line emission of the inner 20AU of stationary and viscous protoplanetary disks and discuss possible reasons for the discrepancies between theoretical and observed spectra.



Artist conception, credits: NASA/JPL-Caltech

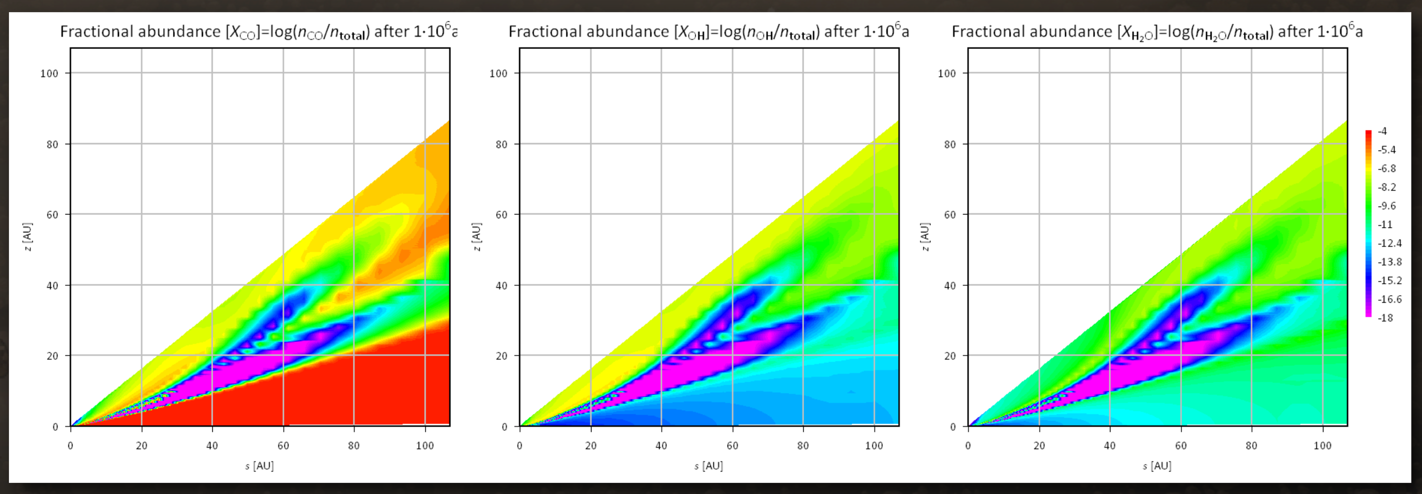
Disk model

- axisymmetric, stationary α-disk (Nomura et al. 2007) around T Tauri star
- gas temperature and density calculated assuming hydrostatic balance and local thermal balance of heating and cooling
- dust temperature derived self-consistently by solving the 2D radiative transfer equation (Dullemond and Turolla 2000, Nomura 2002)
- dust and gas well mixed with constant dust-to-gas ratio 0.01



Chemical network

- UMIST Database for Astrochemistry (Millar et al. 1997): 209 species, connected by 2960 reactions, evolution over one million years
- photodissociation of molecules in the upper layers and close to the star by UV photons, X-rays and cosmic rays
- freeze-out of molecules onto dust grains in cold regions
- consideration for accretion motion currently under development



Molecular emission lines

- parallel line-of-sight integration for mid-infrared emission
- continuum emission from central star and dust; dust absorption and emission calculated using the Jena tables (Ossenkopf & Henning 1994)
- molecular data taken from the HITRAN database (Rothman et al. 2005)
- level populations calculated in local thermal equilibrium
- spectra show CO and OH in emission, but H_2O in absorption; CO_2, HCN and C_2H_2 not detected
- results stand in contrast to observed spectra of young PPDs

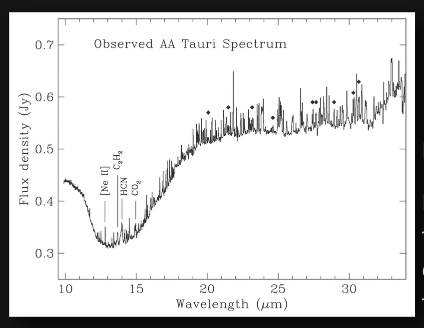
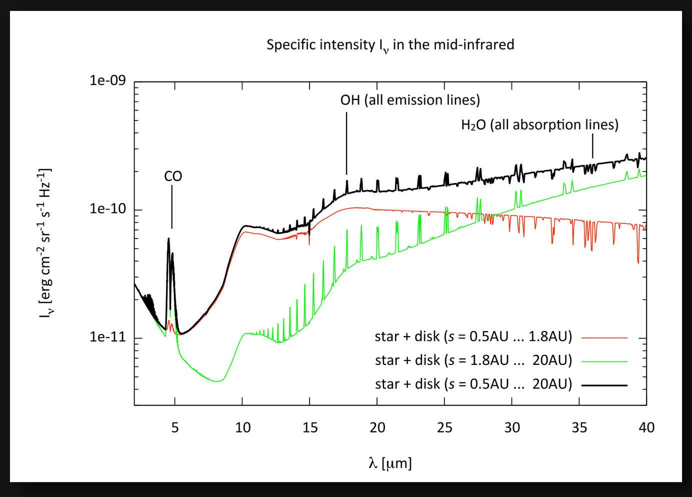


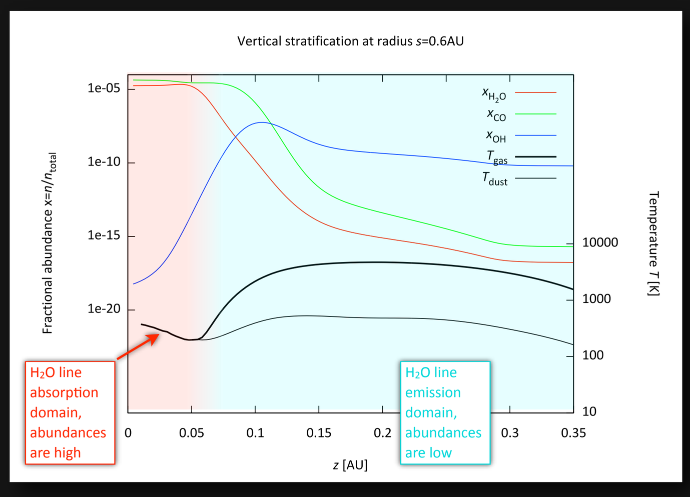
Fig. 1 from Carr & Najita (2008)

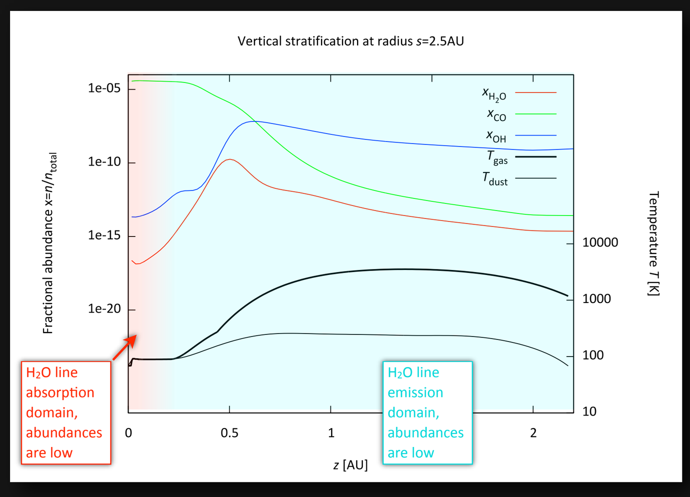
Diamonds mark rotational transitions of OH, unlabeled emission lines are rotational transitions of H_2O



Discrepancies between our model & observations

- inner disk region: water abundances high close to the disk mid plane (line absorption region), but low in upper layers (line emission region)
- inward transport of molecules by accretion, including evaporation from dust particles, may enhance the H_2O abundances in the upper layers
- likewise, vertical (and radial) turbulent mixing may transport H_2O and other molecules into the line emission regions





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