Radiative transfer modeling on AU-Scales of Infrared Molecular Lines from Protoplanetary Disks

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Molecules in the inner regions of regions of protoplanetary disks

In addition to H$_2$, OH, CO, and H$_2$O observed in the NIR, Spitzer detected molecules in the MIR (Carr & Najita 2008, Salyk et al. 2008)

- Most lines are H$_2$O
- OH lines are marked by ♦
- Some lines of C$_2$H$_2$, HCN, and CO$_2$ are marked
- Lines arise from warm gas (500-1000 K) inside 2 AU
- More complex molecules are expected to be found in planet-forming regions
Dust radiation transfer

Dust temperature and mean intensity are calculated (RADMC; Dullemont & Dominik 2004)

Non-LTE excitation calculation

Level populations of molecule are calculated (beta3D; Poelman & Spaans 2005, 2006)

Ray-tracing

Spectrum or image of object is rendered (RADLite; Pontoppidan et al. 2009)
Sub-sampling in each grid cell resolves lines with small intrinsic line widths in regions with large velocity gradients:

- I.e., inner regions of protoplanetary disks

Common codes:
- Integrate across grid cell boundaries
- Narrow lines may be missed
Optimization of RADLite:

- Defines a large number of closely spaced rays
- Thousands of lines are efficiently rendered due to the single integration of continuum rays
- A spectrum and image velocity cube of a line at 3 km s\(^{-1}\) resolution is rendered in 15-30 seconds on a single 3 Ghz Intel Xeon processor
CO ro-vibrational bands

- Spectra at $68^\circ$ and $72^\circ$ inclination angles
- Both absorption and emission components are shown
- Models spatial scales below 0.1 and > 100 AU and spectral ranges from < 0.1 km s$^{-1}$ to the entire spectrum
- Dynamic ranges of 4 – 5 orders of magnitude can be treated simultaneously
Beta3D

\[
\beta_{ul}(x, y, z, k) = \frac{1 - \exp(-\tau_{ul}(x, y, z, k))}{\tau_{ul}(x, y, z, k)}
\]

- Grid cells interact with each other (Poelman & Spaans 2005, 2006)
- Suitable for arbitrary geometries and any atom & molecule
- 10 – 100 times fast than existing MC/ALI codes especially at high optical depths
Non-LTE/LTE column density ratios

- LTE approximation is only valid at small radii.
- Sub-thermal decrease in column density is larger for levels with a higher excitation energy.
- Ground vibrational level (black) deviates from LTE at higher level energies than first vibrational level (red).
Fiducial model

- Freeze-out onto grains can significantly reduce the amount of water in the gas phase
- Gas temperature in the disk surface is decoupled from dust, due to heating by FUV and/or X-rays
- Gas to dust ratio is larger than the canonical ISM value of 160 due to dust settling
Vertical cold finger effect

- Static chemical models predict a lowered water abundance below $T \sim 300$ K
- Higher depletions are necessary due to high optical depths
- Proposal: water is transported below the snow-line and freezes out, and will take part in settling to mid-plane (variation of Stevenson & Lunine 1988 radial cold finger effect)
Non-LTE  Low spectral resolution: $\lambda/\Delta\lambda=600$ (500 km/s)  LTE

Constant abundance
Freeze-out added
Gas decoupling added
Gas/dust ratio increased
Vertical cold finger effect added
Comparison to observations

• Comparison to observations of AA Tau, DR Tau, and AS 205 (Carr & Najita 2008, Salyk et al. 2008)

• No attempt is made (yet!) to match observations

• A full parameter study is in preparation (Meijerink et al.)
Full range infrared water spectrum from a typical protoplanetary disk
• RADLite renders a large number of molecular lines, e.g., CO and H$_2$O

• A water spectrum (~1000 lines) in the infrared (2-200 $\mu$m) at 3 km s$^{-1}$ resolution takes 1-2 hours on a single workstation

• The code has applications to chemical and excitation models as well as observations from infrared spectrometers

• Infrared spectroscopy of disks in the N-band has not received much attention is due to a sensitivity deficit $\rightarrow$ remedied by E-ELT
Summary (part 2)

• Non-LTE treatment is crucial in determining the molecular distributions

• An increase of the gas-to-dust ratio from the canonical value of $\sim 100 – 200$ is essential in order to approach the observed line strengths and line-to-continuum ratios

• The predicted lower limit to the water abundance in cold regions still produces too much emission

• A vertical cold finger effect is proposed to further lower the abundance

• Current study is qualitative at this time