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

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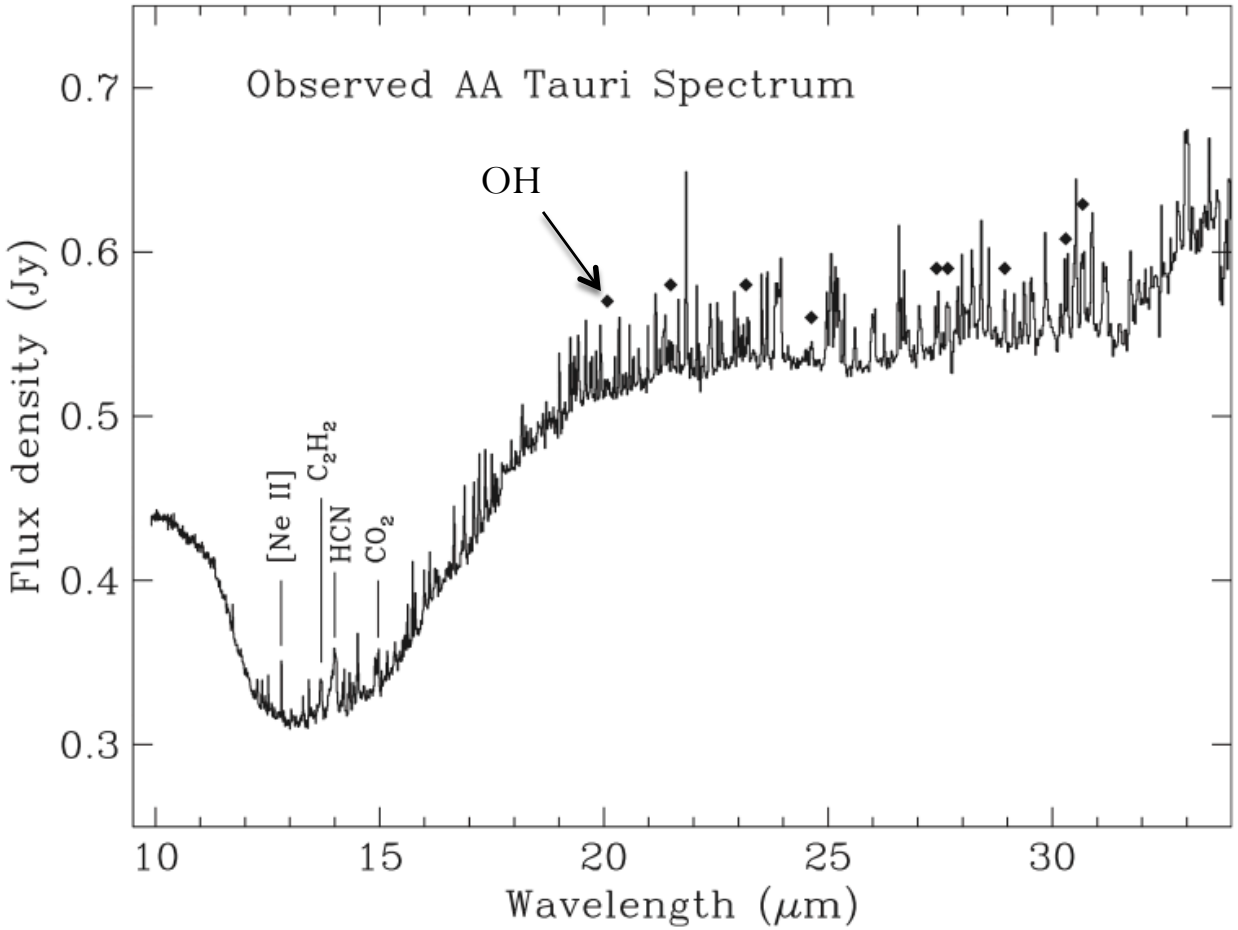
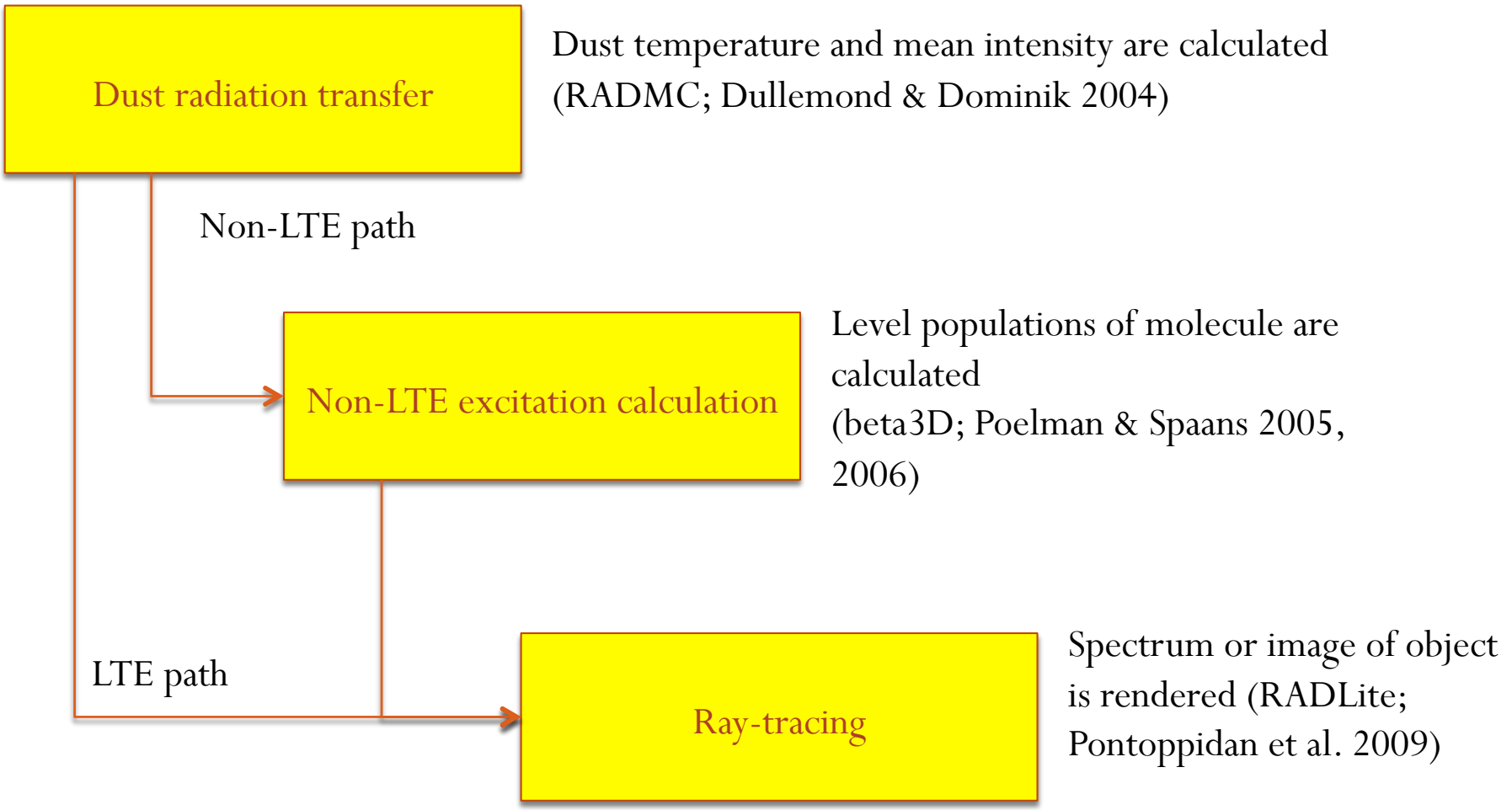
# Molecules in the inner regions of regions of protoplanetary disks

In addition to $H_2$, OH, CO, and $H_2O$ observed in the NIR, Spitzer detected molecules in the MIR (Carr & Najita 2008, Salyk et al. 2008)

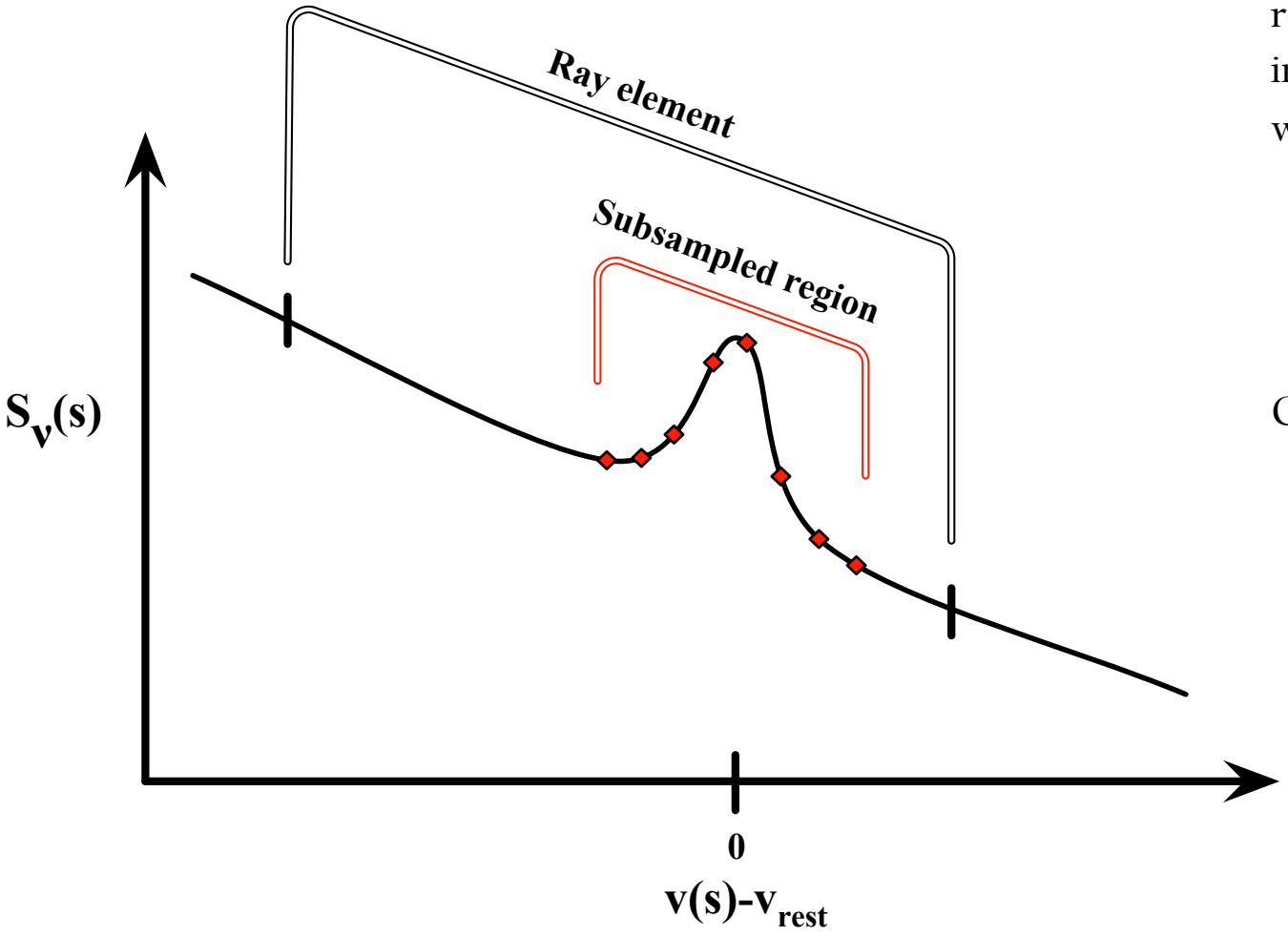



- Most lines are $H_2O$
- OH lines are marked by ◆
- Some lines of $C_2H_2$, HCN, and $CO_2$ are marked
- Lines arise from warm gas (500-1000 K) inside 2 AU
- More complex molecules are expected to be found in planet-forming regions

# Flow chart of the codes



# RADLite



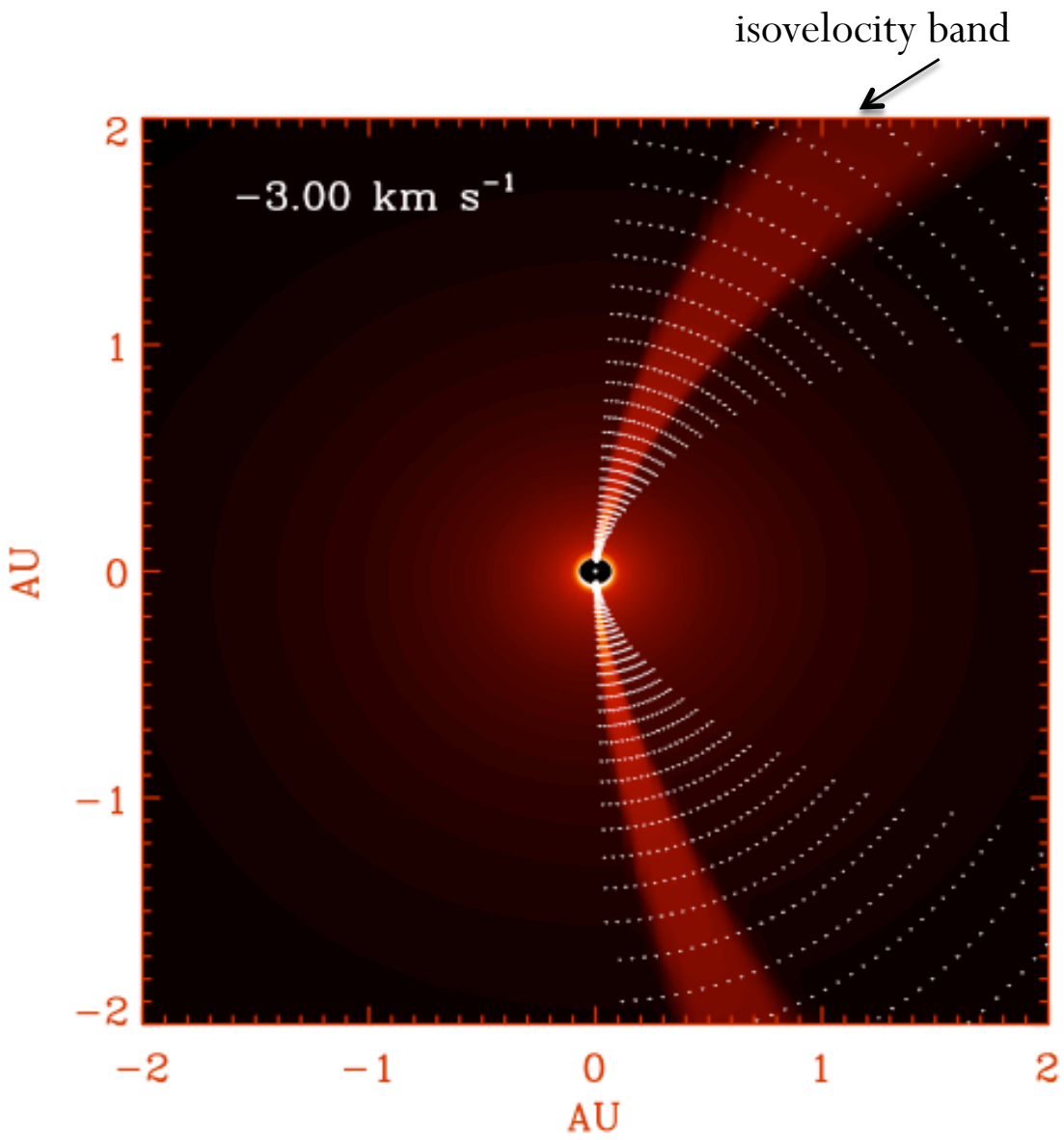

Sub-sampling in each grid cell resolves lines with small intrinsic line widths in regions with large velocity gradients:

- I.e., inner regions of protoplanetary disks

Common codes:

- Integrate across grid cell boundaries
- Narrow lines may be missed

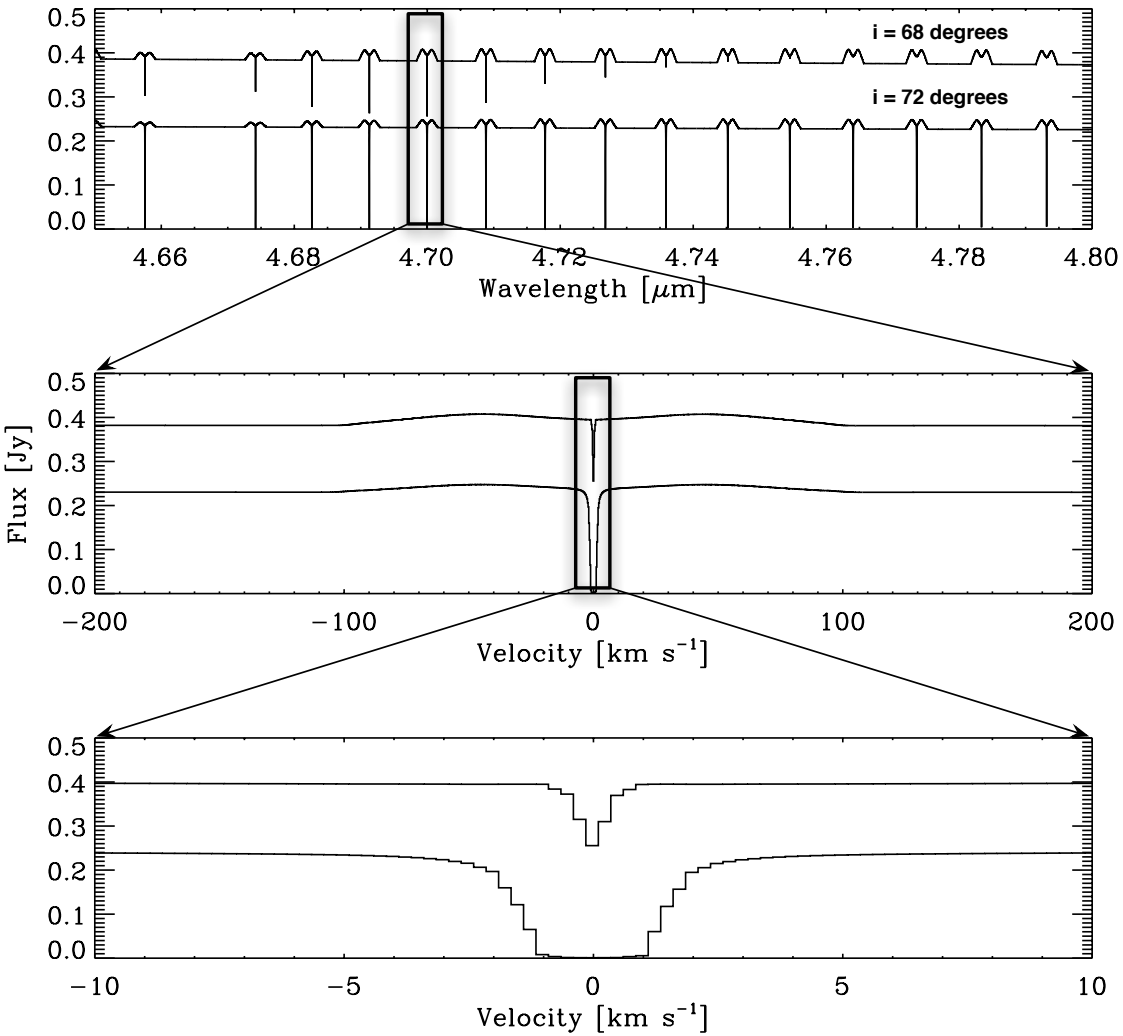
# Optimization of RADLite




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

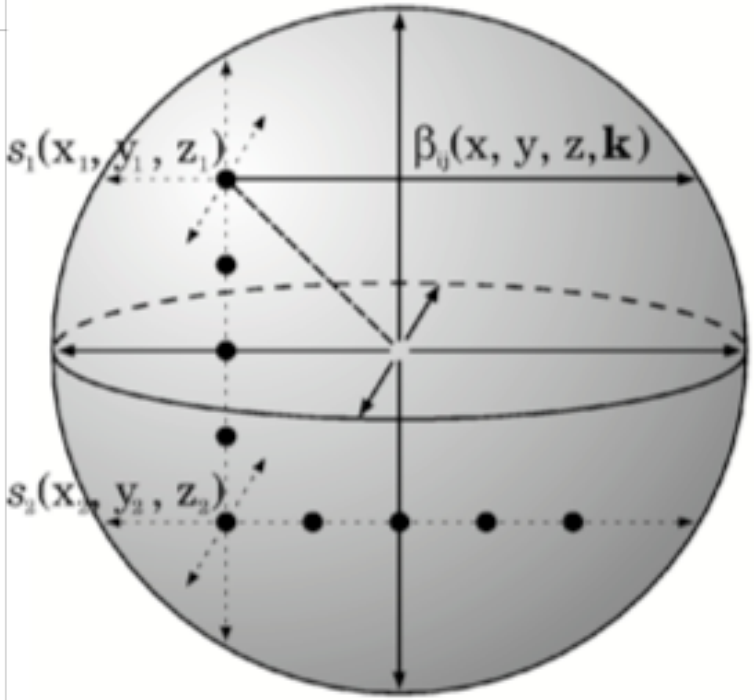



- Spectra at 68° and 72° inclination angles
- Both absorption and emission components are shown
- Models spatial scales below 0.1 and > 100 AU and spectral ranges from < 0.1 km $s^{-1}$ to the entire spectrum
- Dynamic ranges of 4 – 5 orders of magnitude can be treated simultaneously

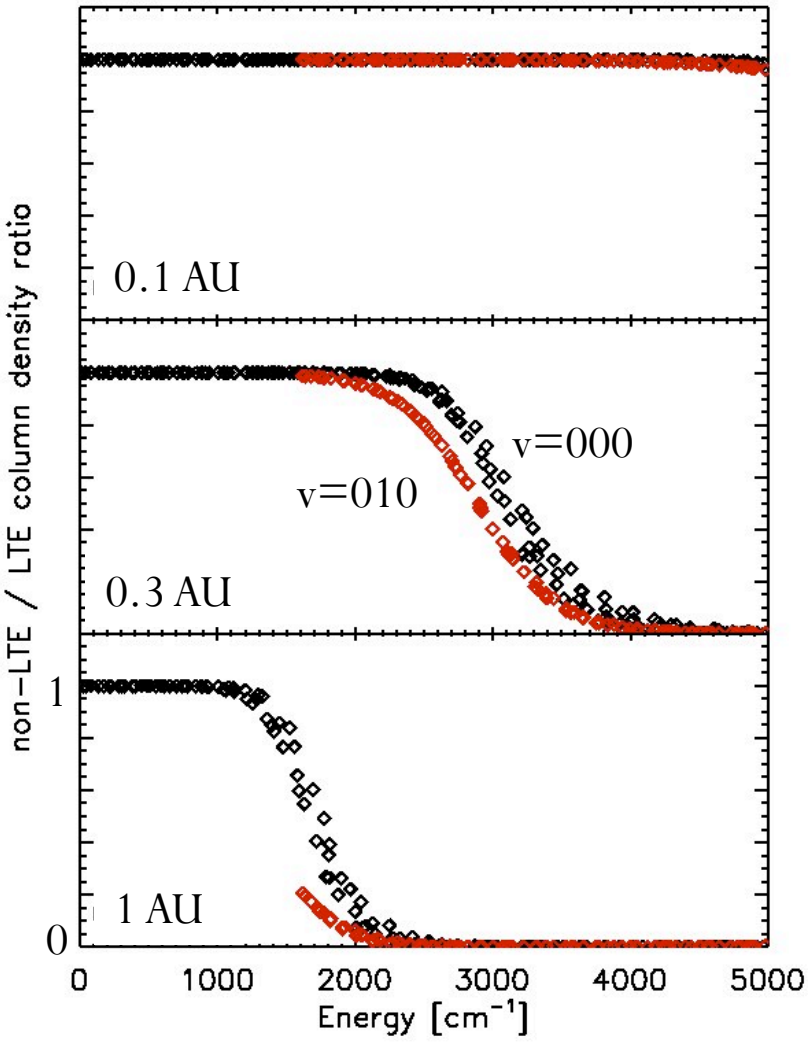
# Beta3D

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

- 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

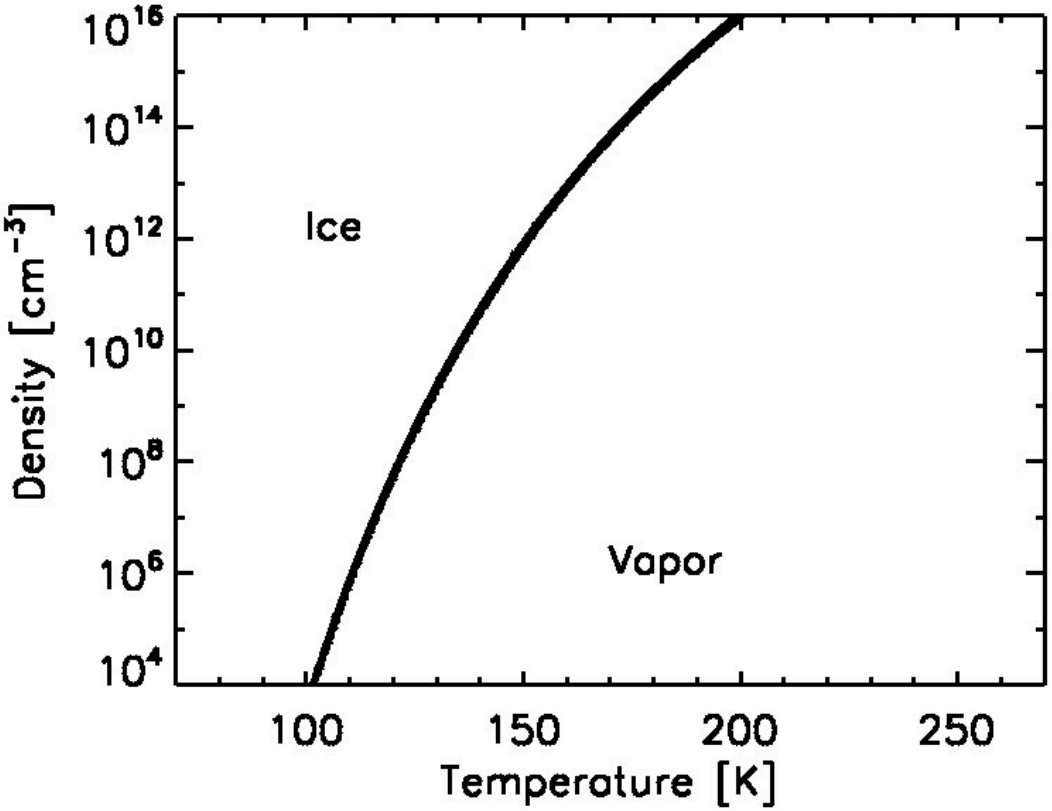


# Non-LTE/LTE column density ratios




- 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)

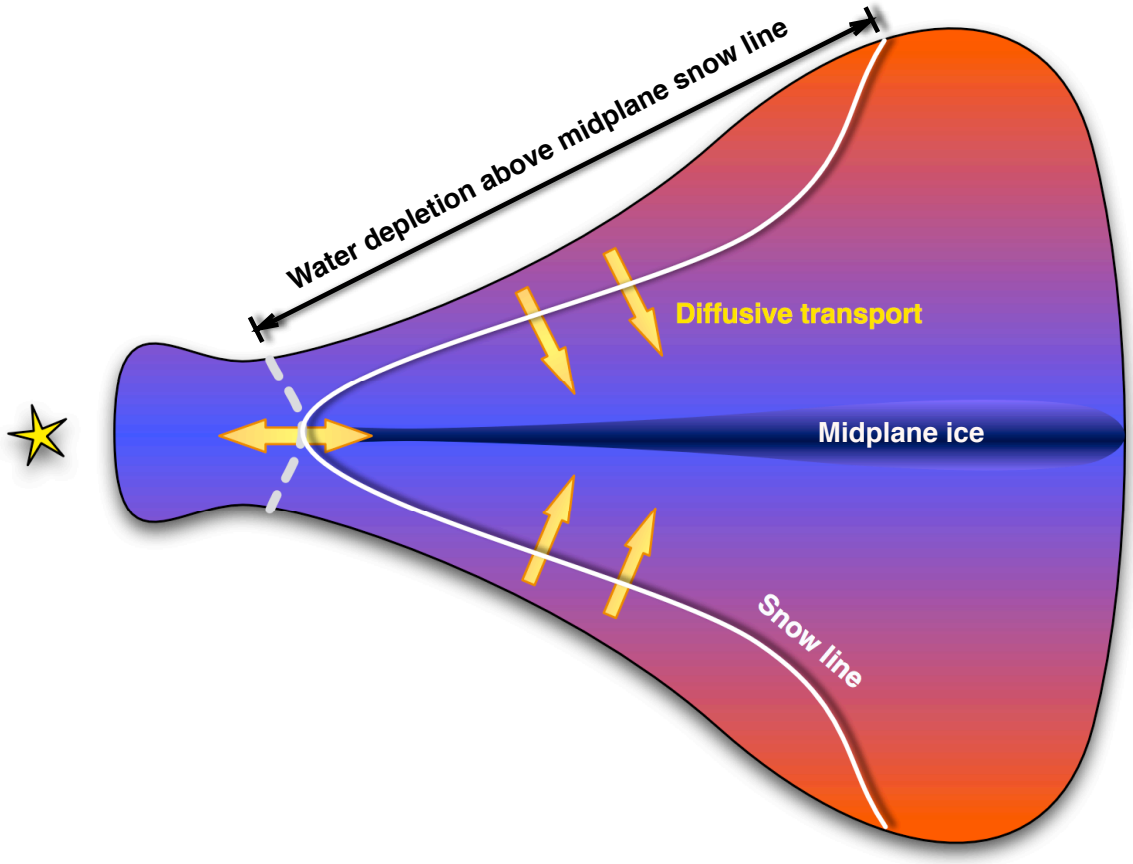
# Fiducial model




- 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 ~ 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)



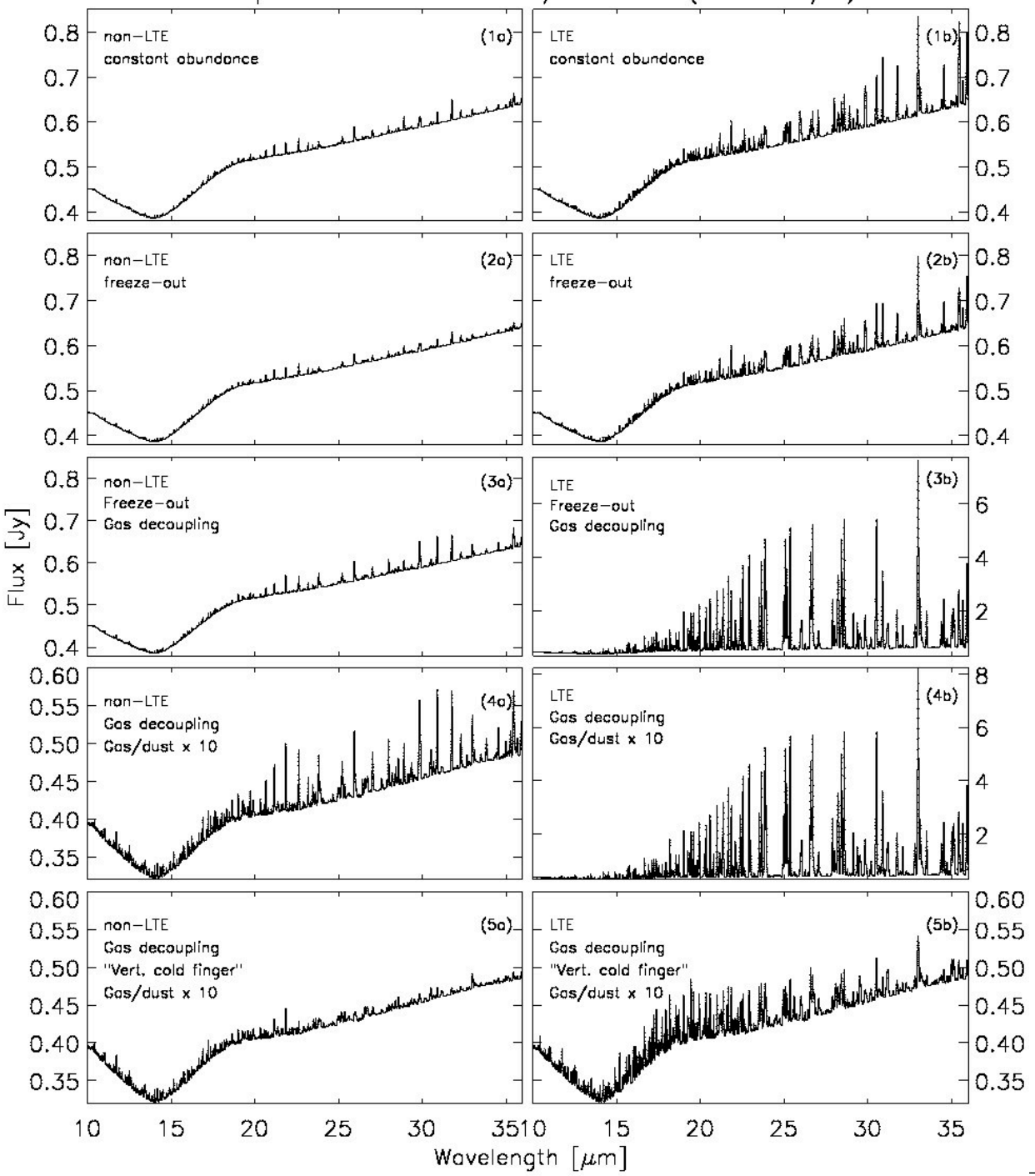
Constant abundance

Freeze-out added

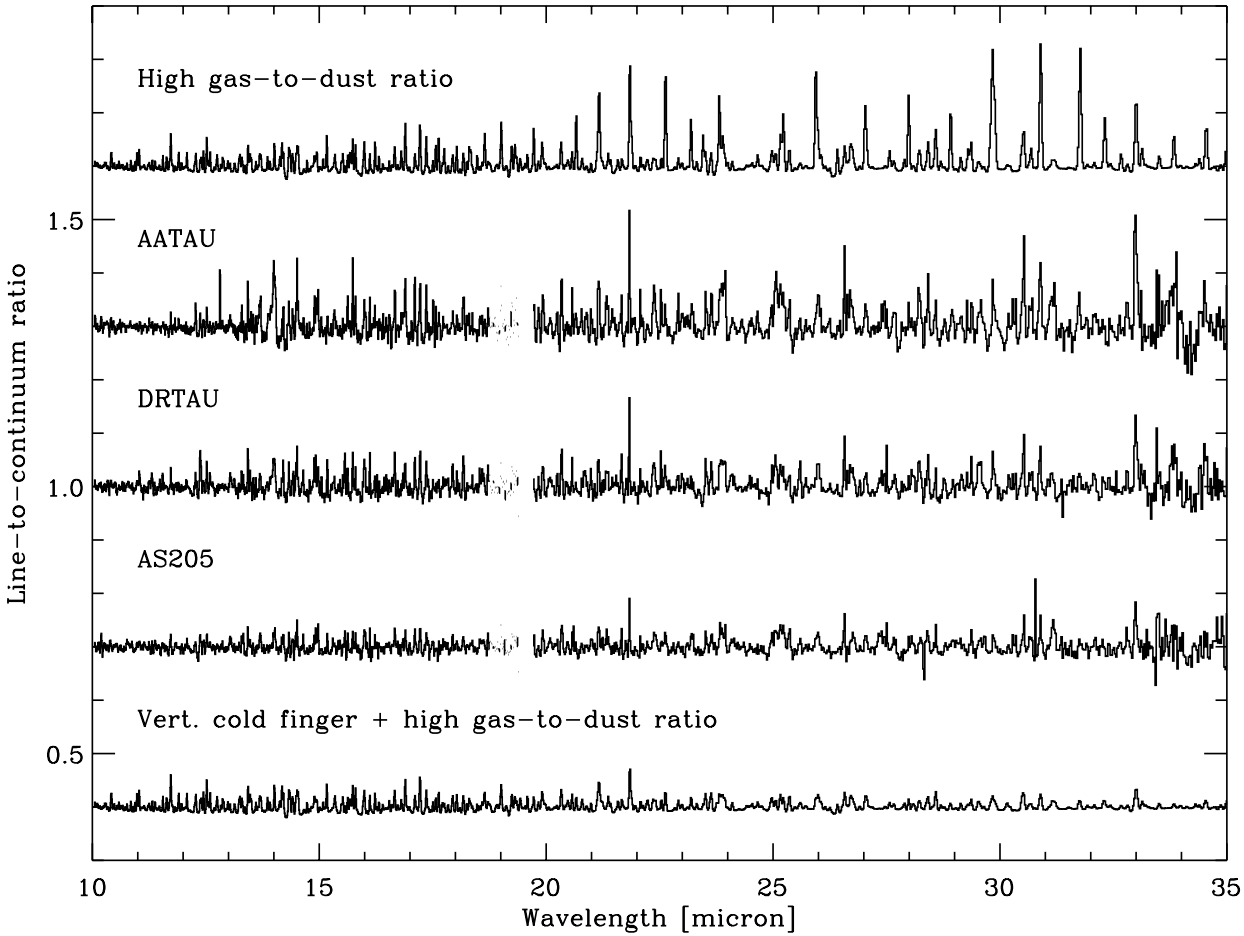
Gas decoupling added

Gas/dust ratio increased

Vertical cold finger effect added

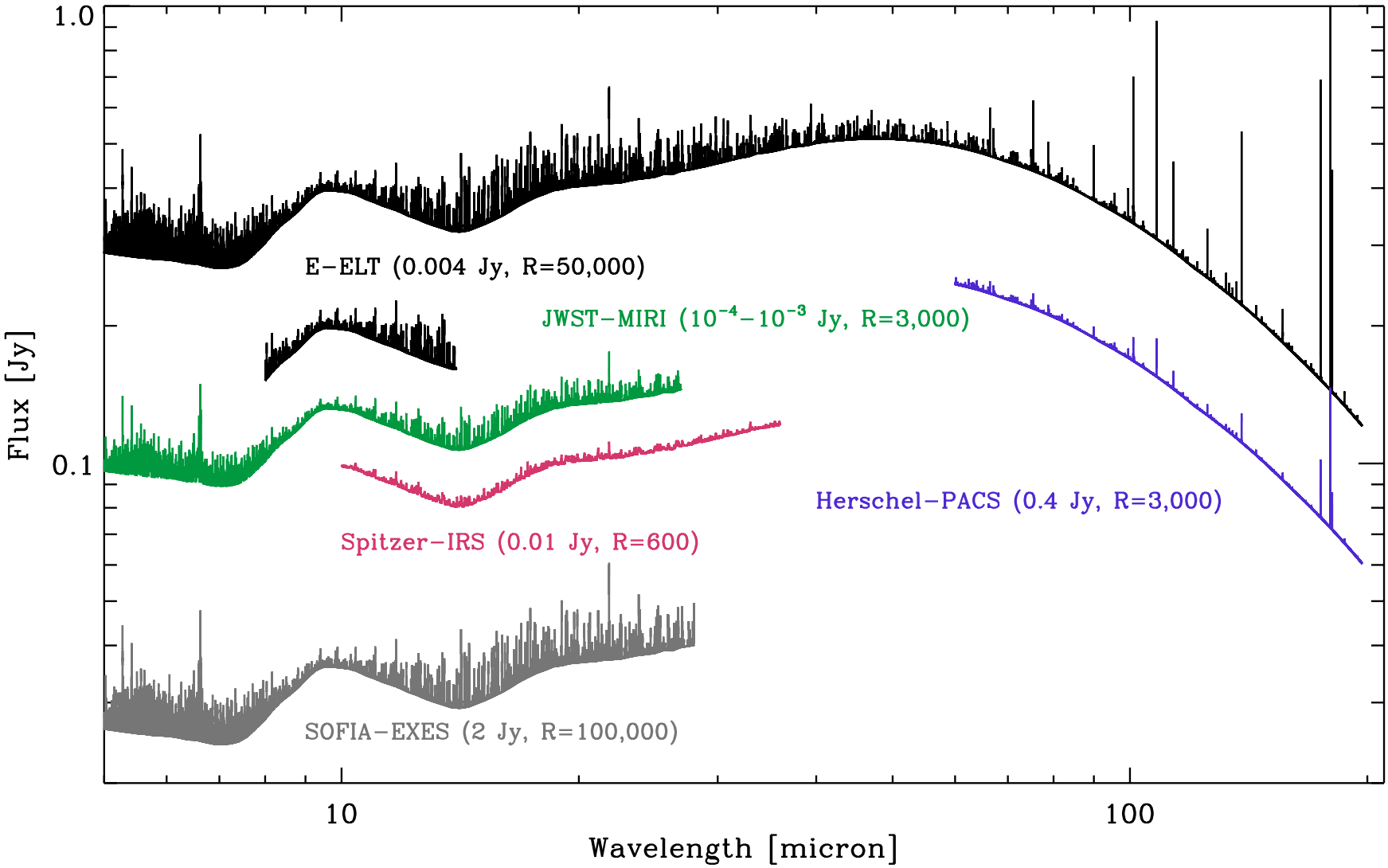


# Comparison to observations




- 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



# Summary (part 1)

- RADLite renders a large number of molecular lines, e.g., CO and $H_2O$
- 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 → 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