The chemical history of ices in protoplanetary disks

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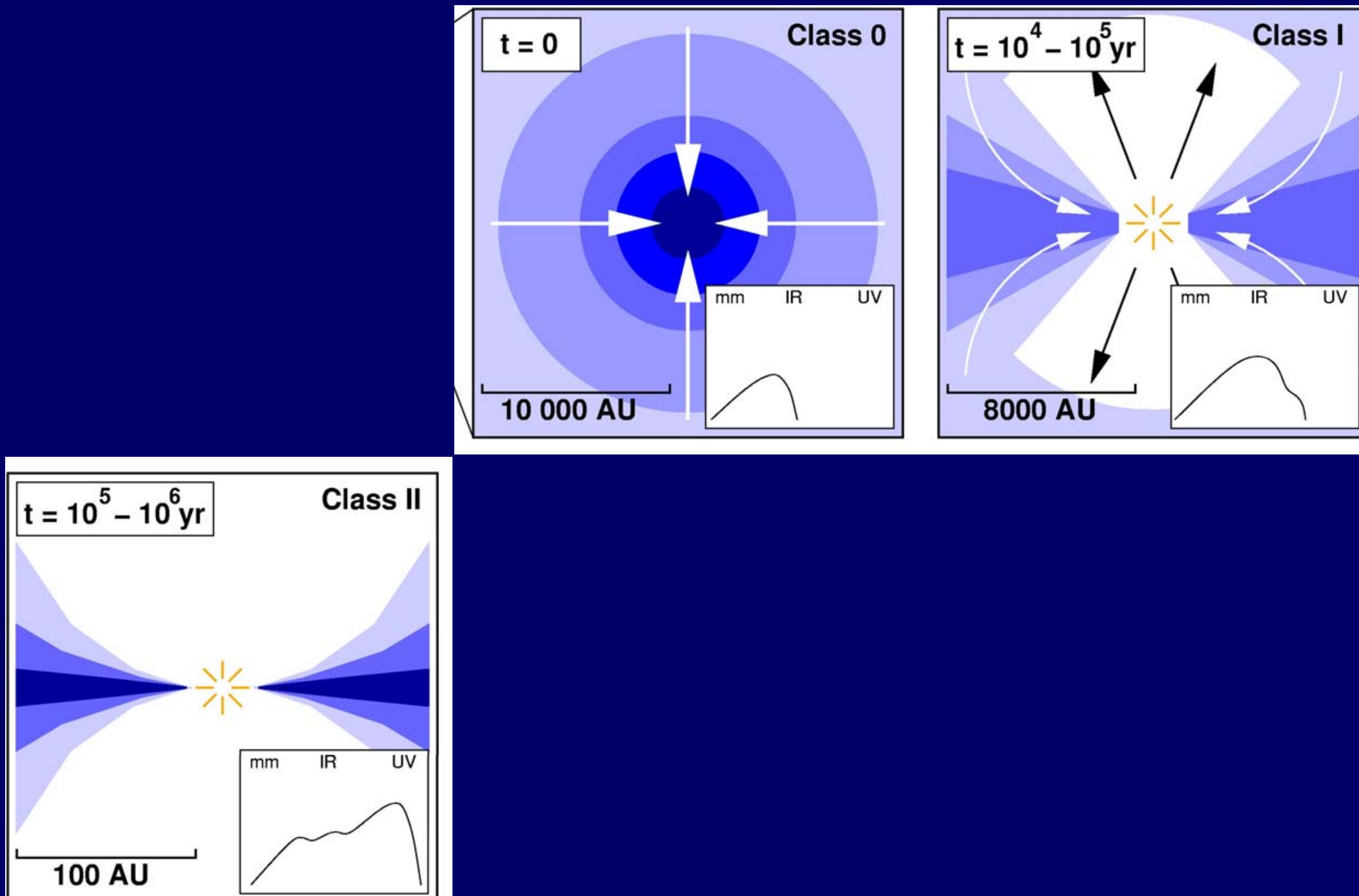
Note for online PDF version:
the results and conclusions presented here are from work in progress and may be different from what is ultimately published as a paper.

Star and planet formation

(low-mass stars)



Jonkheid et al. 2006

Chemical complexity

Key questions

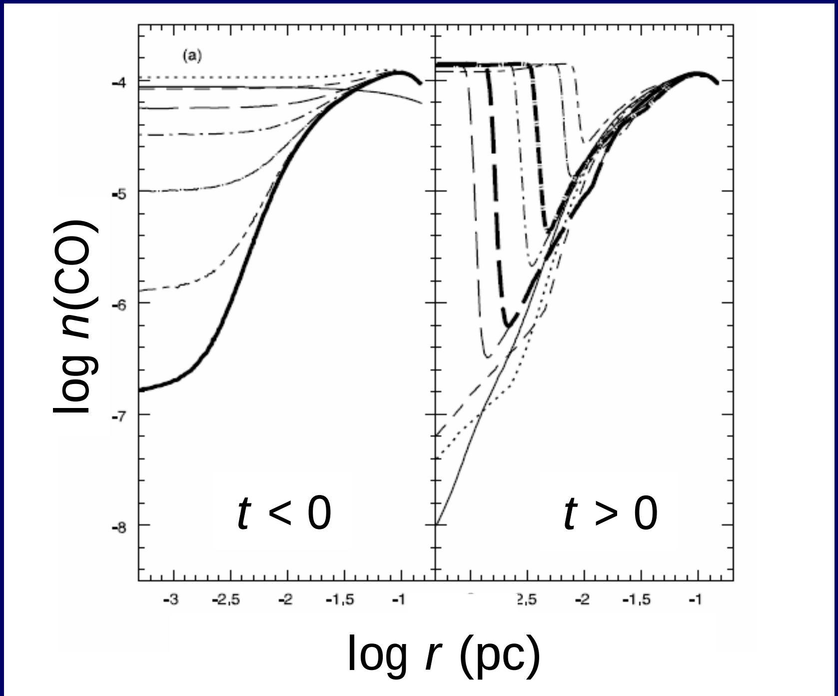
- How does the chemical composition change during formation of a star and disk?
- What is the chemical composition of the building blocks for planets and comets?

Star formation is a chemically complex process

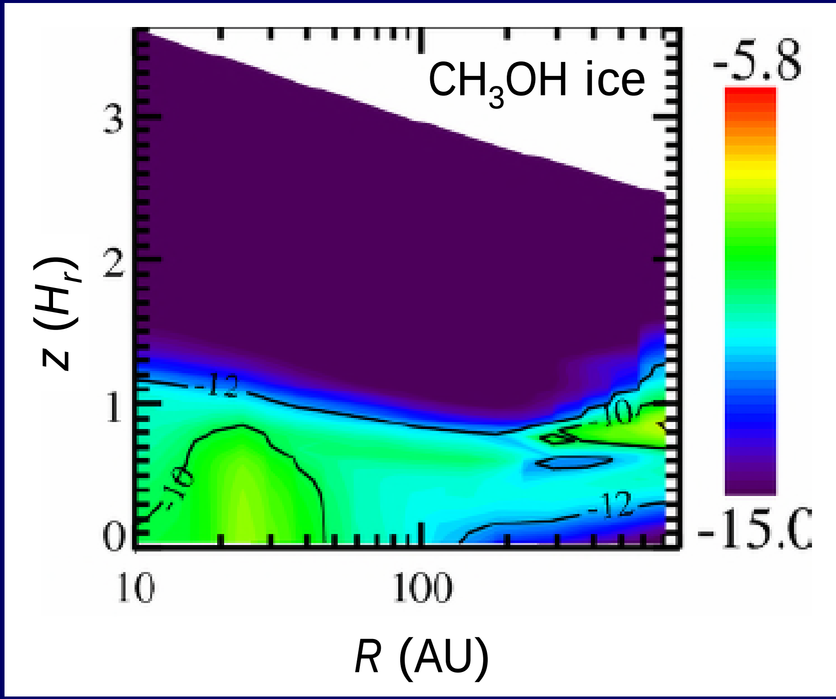
- Where exactly does infalling material end up?
- What is its chemical history?

Earlier work

- 1D collapse model
- No disk



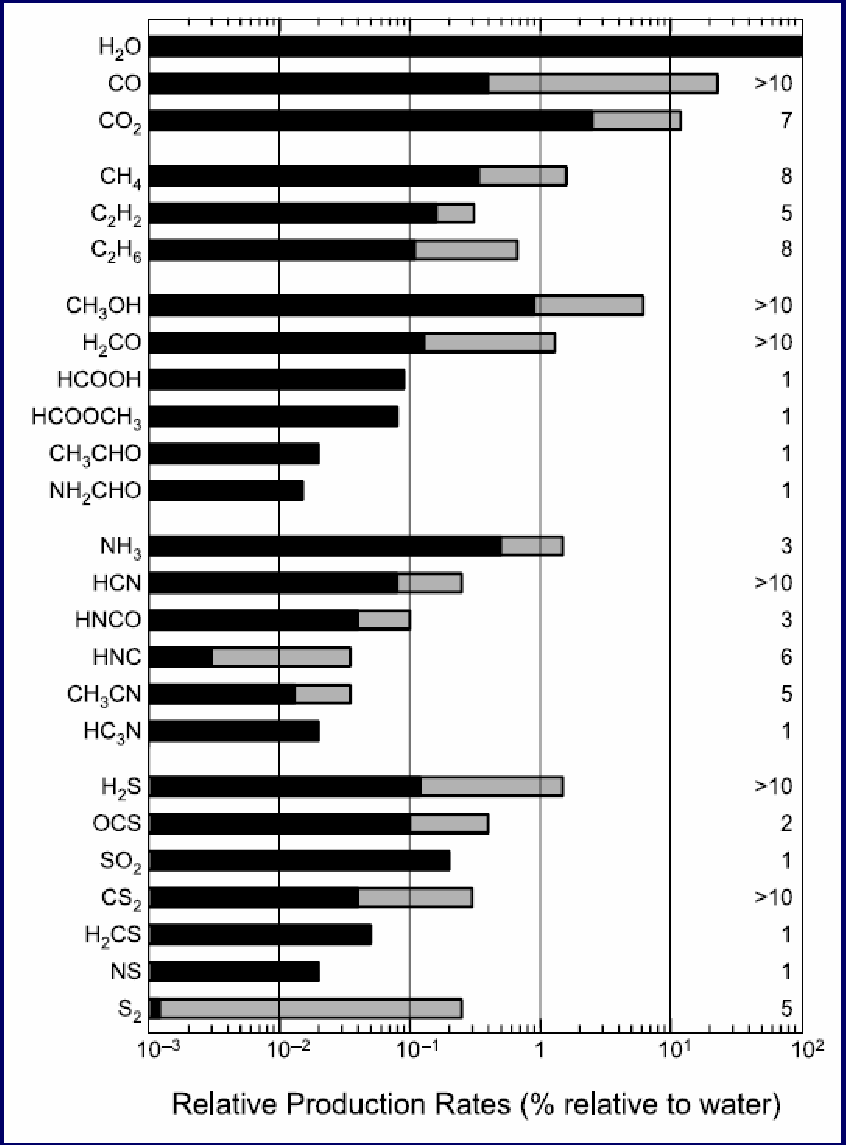
- 2D disk model
- Initial conditions?



Lee et al. 2004, Semenov et al. 2006

Comets: a glimpse at history

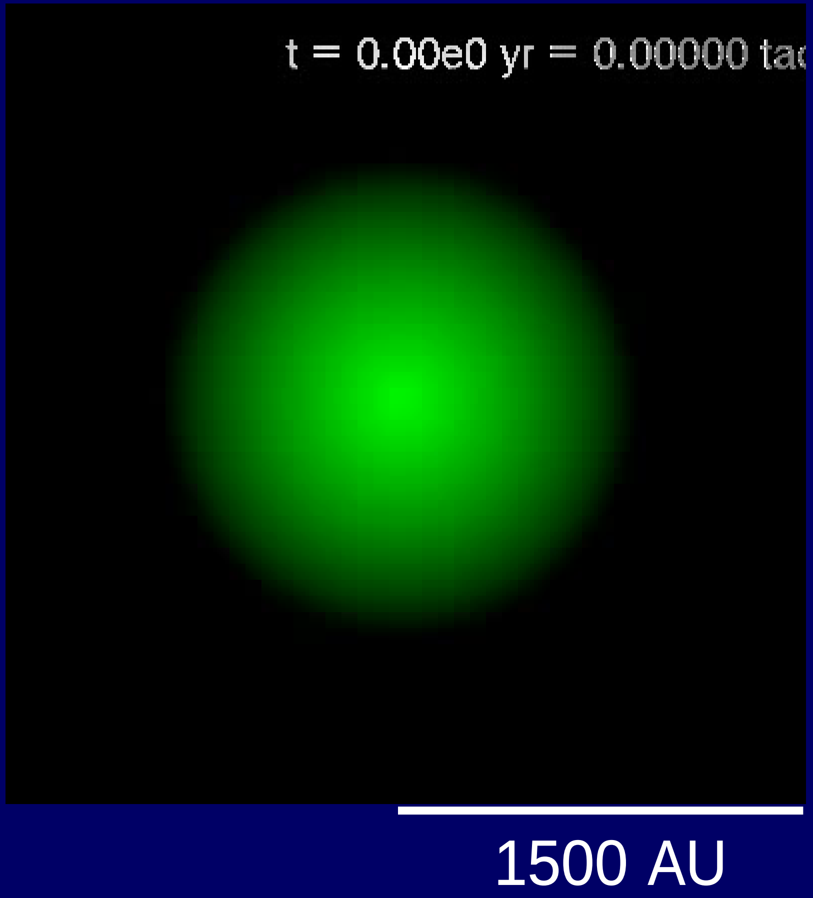
- CO: 0.4—20% of H_2O
- Complex organics also cover large abundance range (not shown)
- Variations remain poorly understood
  → chemical differences during collapse?



Bockelée-Morvan et al. 2004

Analytical star formation model

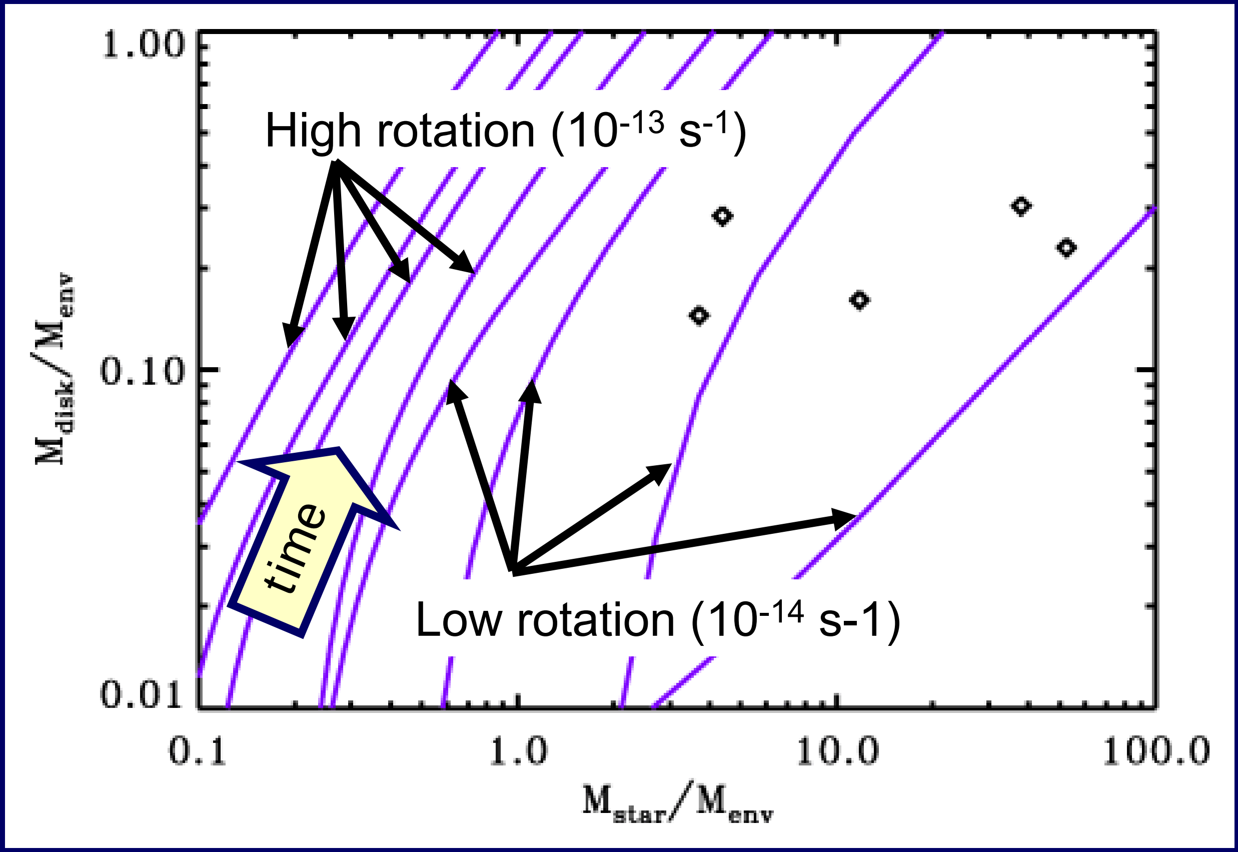
- Density & velocity: inside-out collapse
  Shu (1977),
  Terebey, Shu & Cassen (1984)
- Dust temperature (important!) from full radiative transfer
  (RADMC:
  Dullemond & Dominik 2004)
- Physics compare well with hydro models
  (Brinch, van Weeren &
  Hogerheijde 2008)



Easy to change initial conditions

Model vs. observations: masses

- Lines: model with different initial conditions
- Points: SMA observations

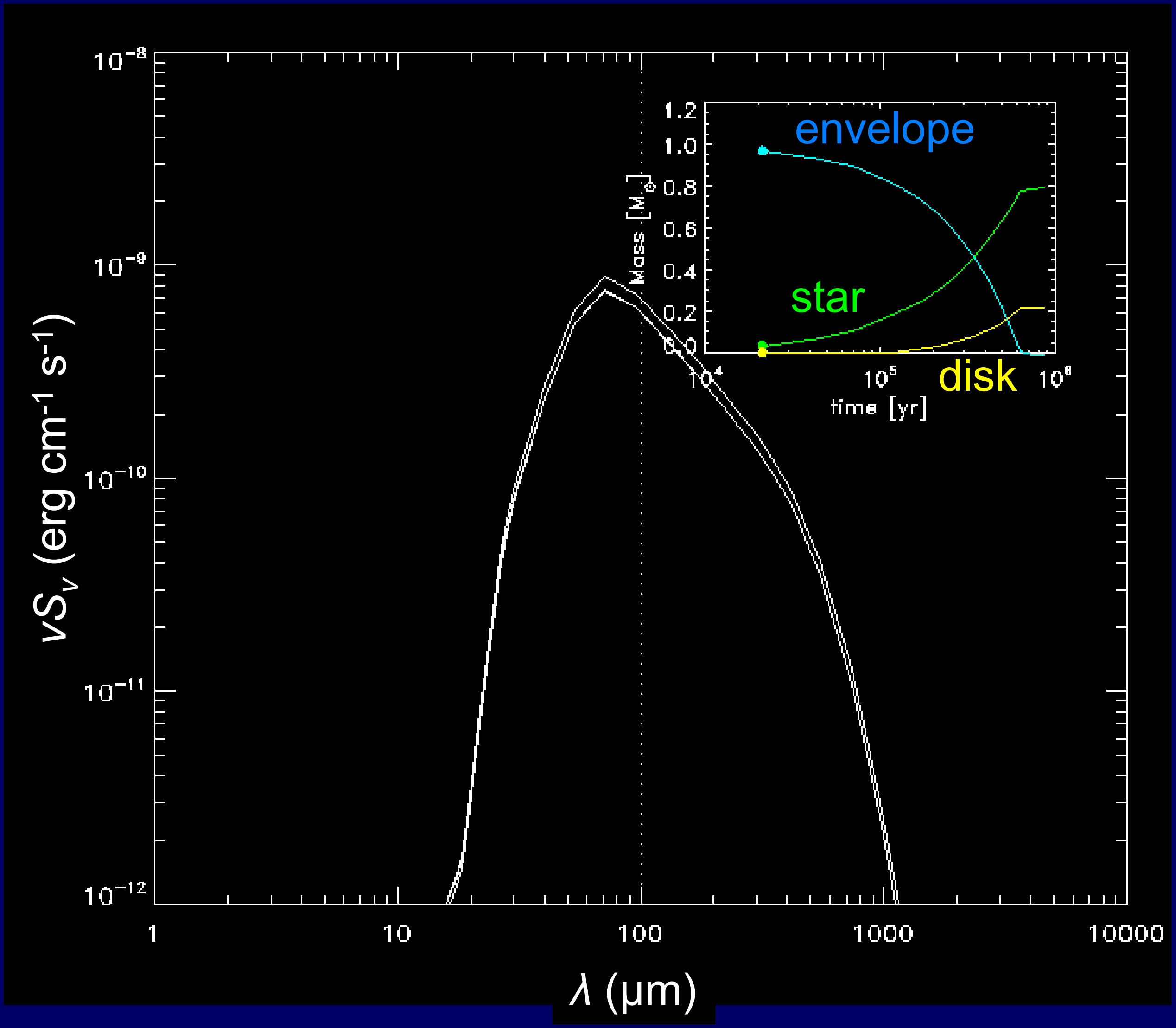


Jørgensen et al. in prep.

Model vs. observations: SED

SED goes from Class 0 to I, but not to II

Redo this for lower M_{disk}

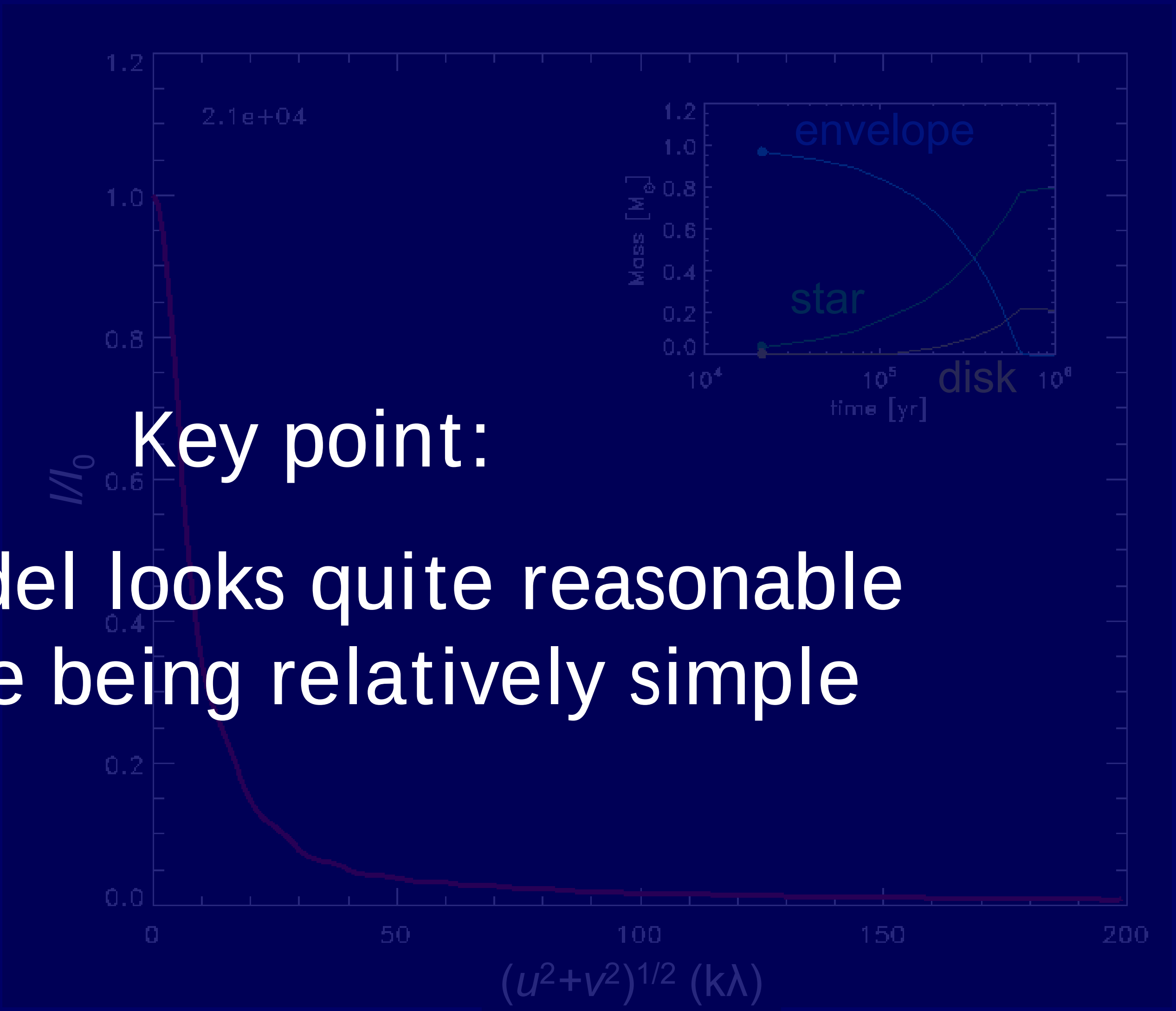


Jørgensen et al. in prep.

Model vs. obs.: interferometry

Envelope/disk break visible from 10^5 yr onwards

Break never becomes very prominent



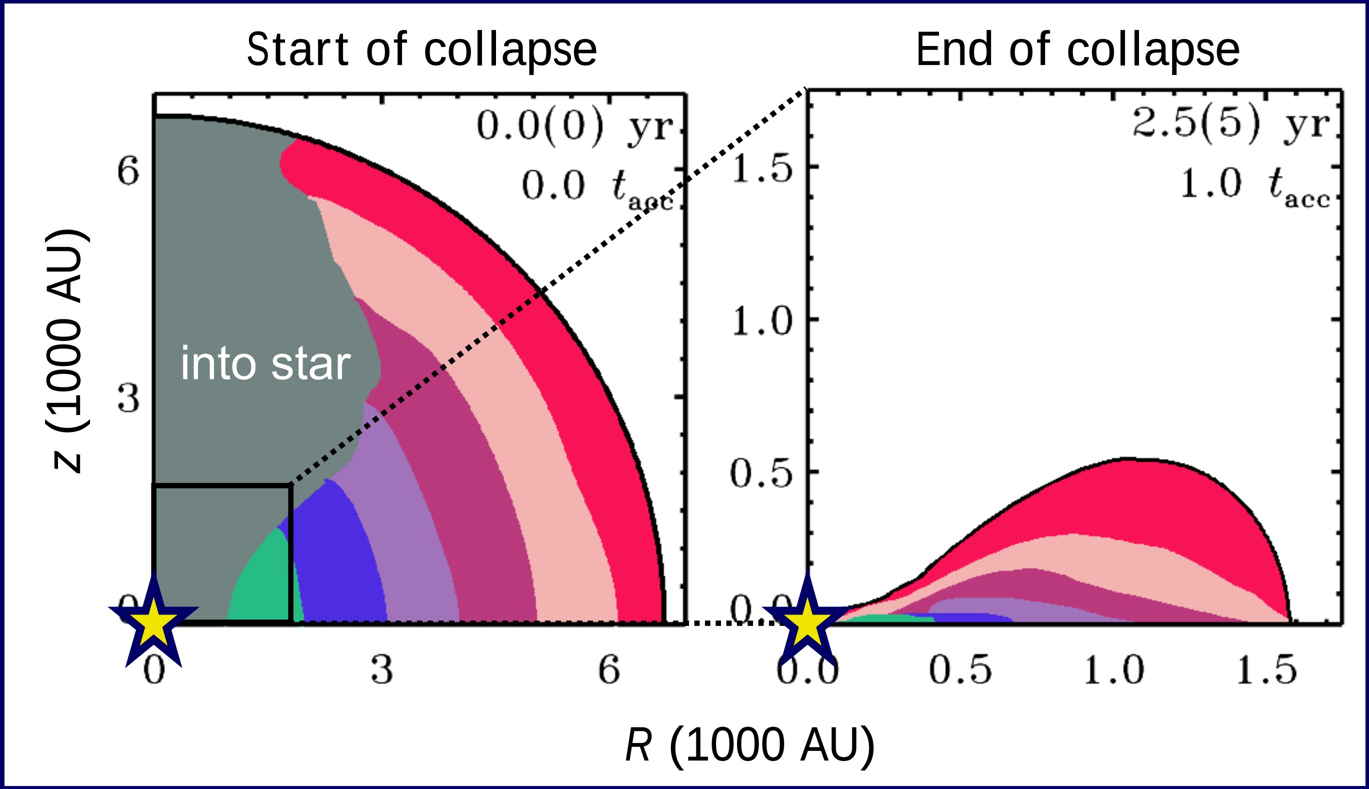
Key point:

our model looks quite reasonable despite being relatively simple

Jørgensen et al. in prep.

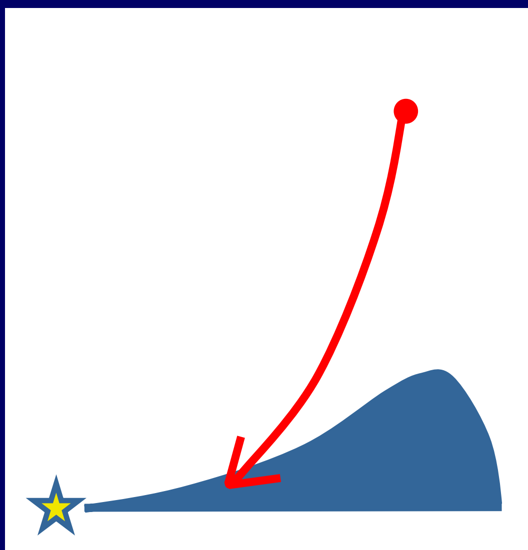
Where does material go to?

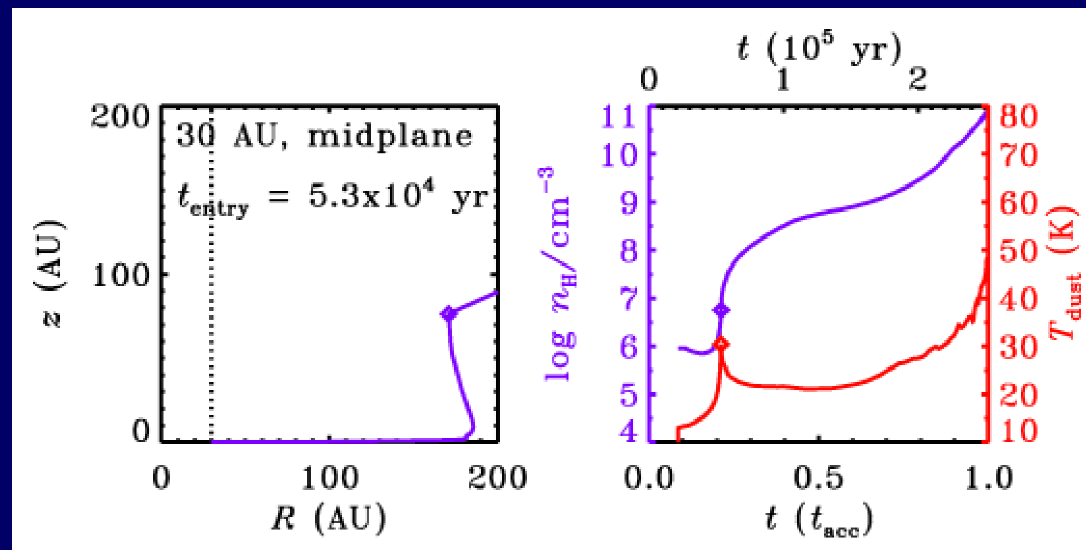
Inside-out collapse gives a layered disk



Follow infalling parcels

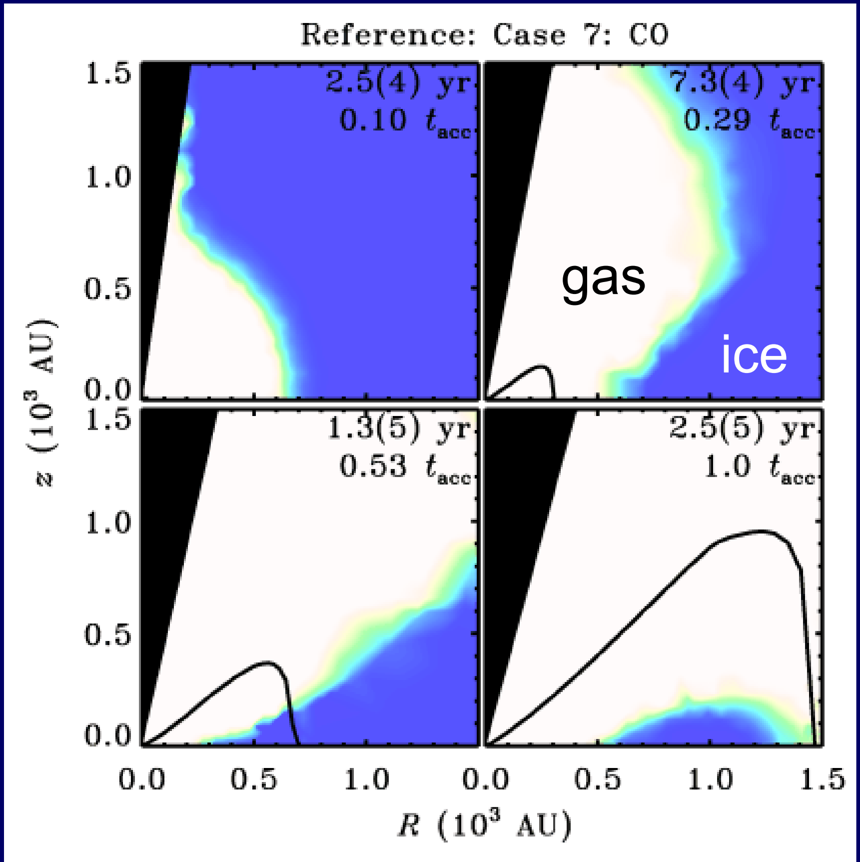
- Need to solve chemistry dynamically: compute *n*, *T* along many trajectories



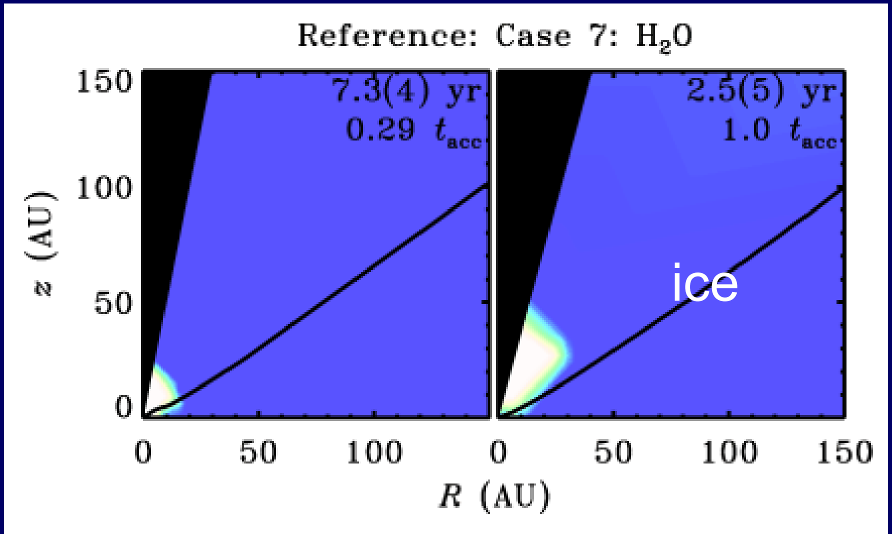


- Jump in *n*, *T* upon entering disk
- *n* increases by factor of ~10^5 overall, *T* goes from 10 to several 10s of K

Gas & ice: pure CO, H_2O



CO



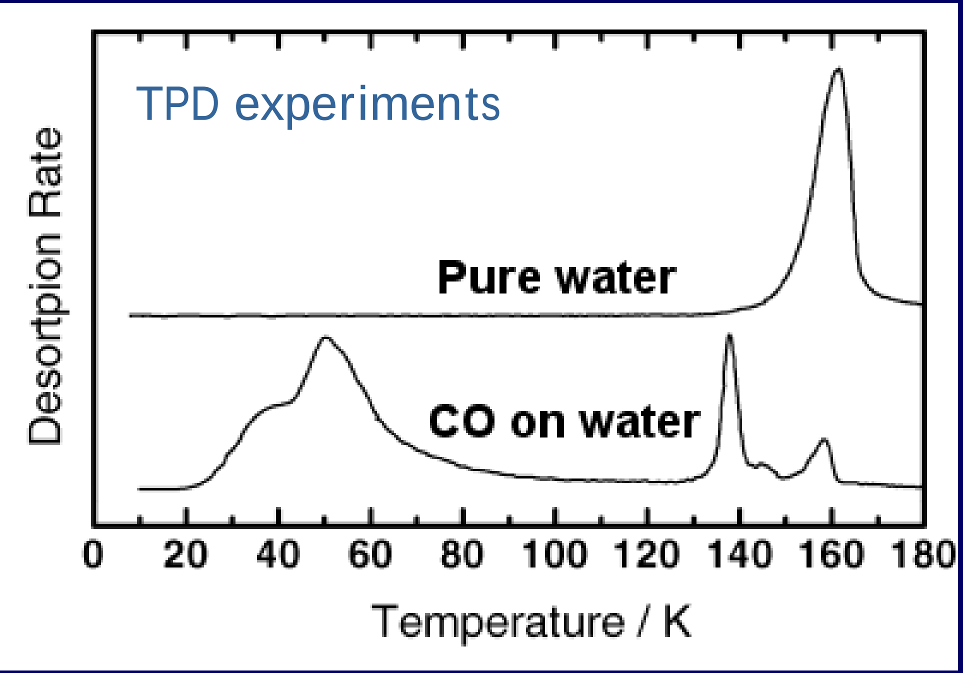
H_2O

blue: all ice
white: all gas
black: outflow
black curve: disk surface

- CO desorbs during infall, re-adsorbs in disk below 18 K
- H_2O remains solid except inner ~10 AU

Closer to reality: ice mixtures

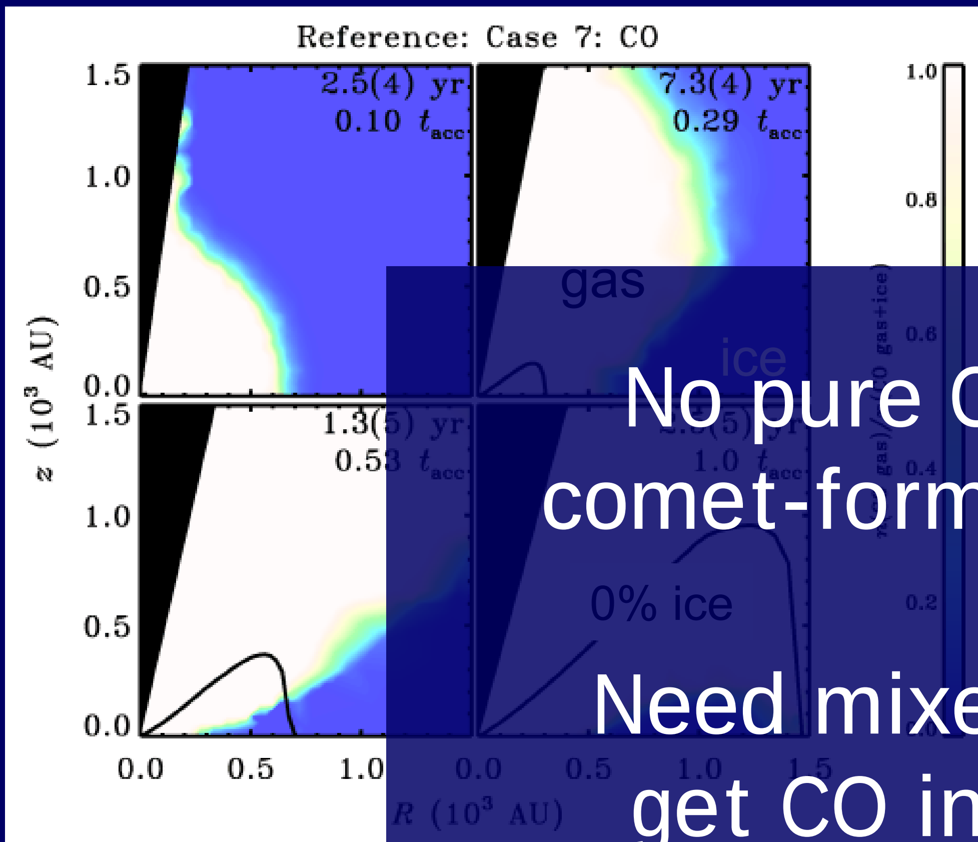
- Real ices in space are mixed
- H_2O most abundant ice → desorption of other ices depends on H_2O
- Depending on binding energy, up to four desorption channels are possible
- We can model this with multiple ice flavours



Collings et al. 2004, Viti et al. 2004

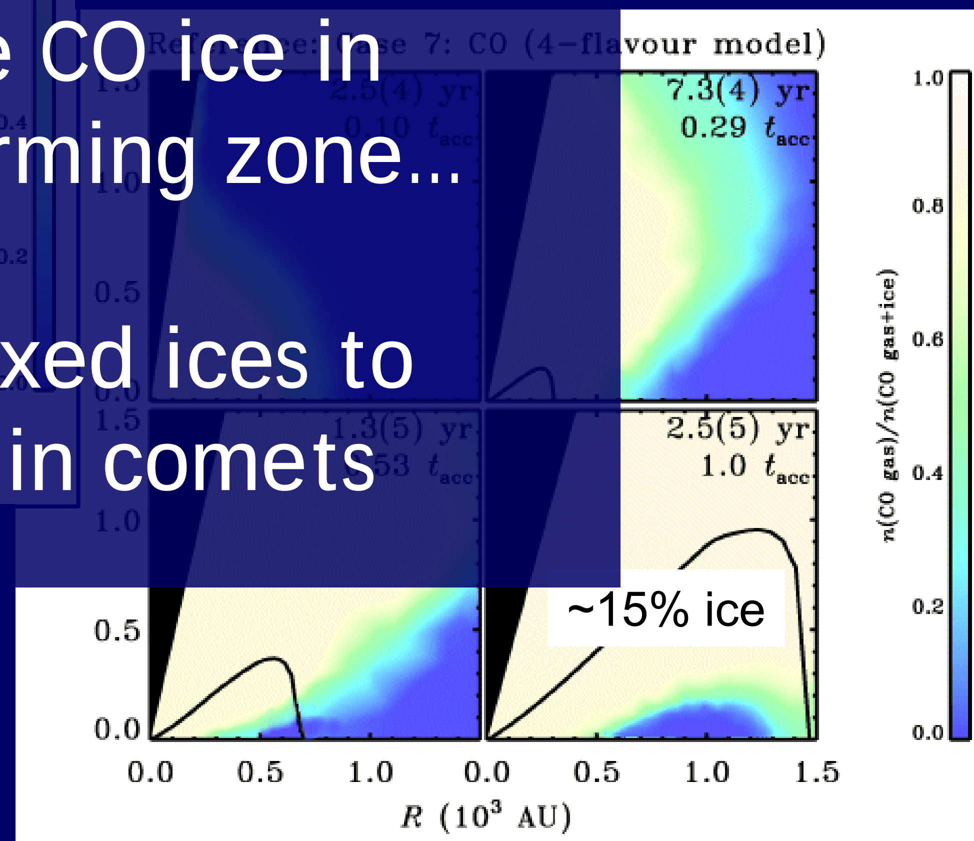
One vs. four flavours of CO

blue: all ice | white: all gas | black: outflow



1 flavour of CO

4 flavours of CO

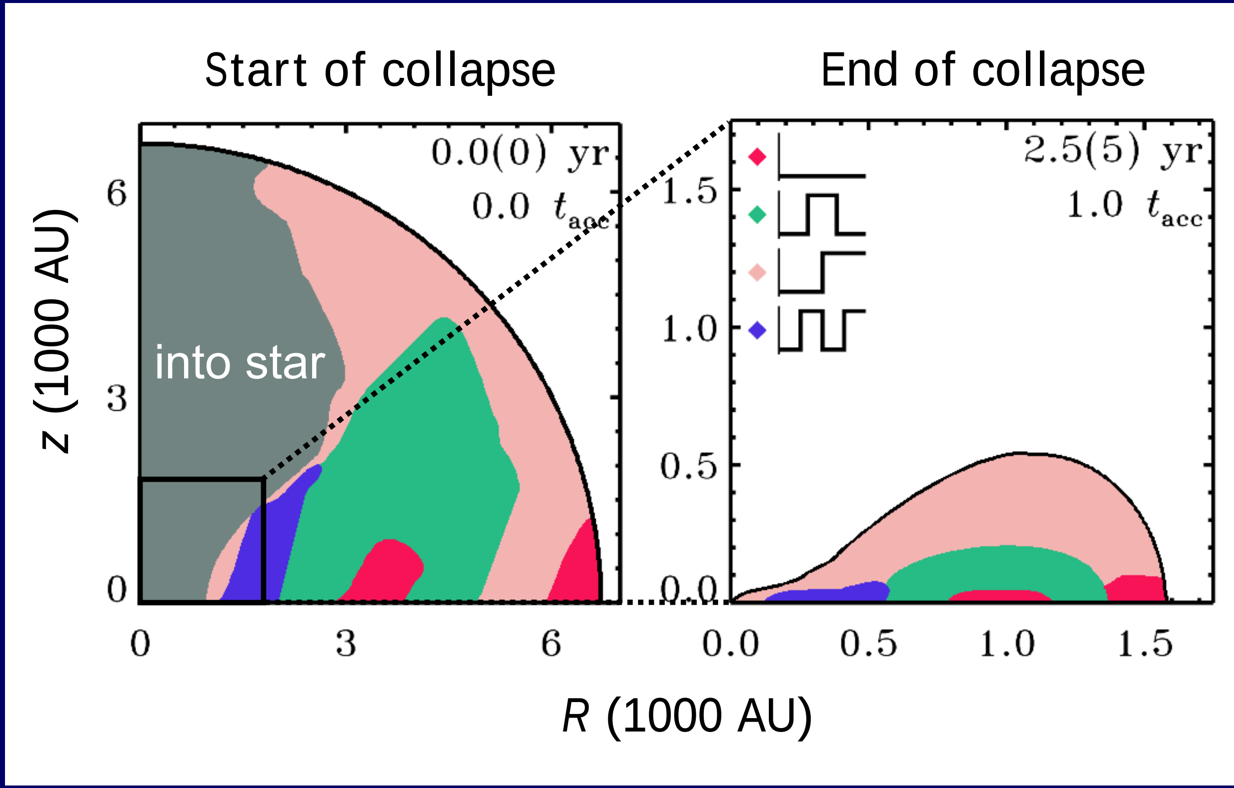


No pure CO ice in comet-forming zone...

Need mixed ices to get CO in comets

Some CO now desorbs at higher temperatures, so the ice fraction is larger

Chemical zones: CO gas/ice



- Red: CO remains adsorbed (pristine!)
- Green: CO desorbs and re-adsorbs
- Pink: CO desorbs and remains desorbed
- Blue: multiple desorption/adsorption

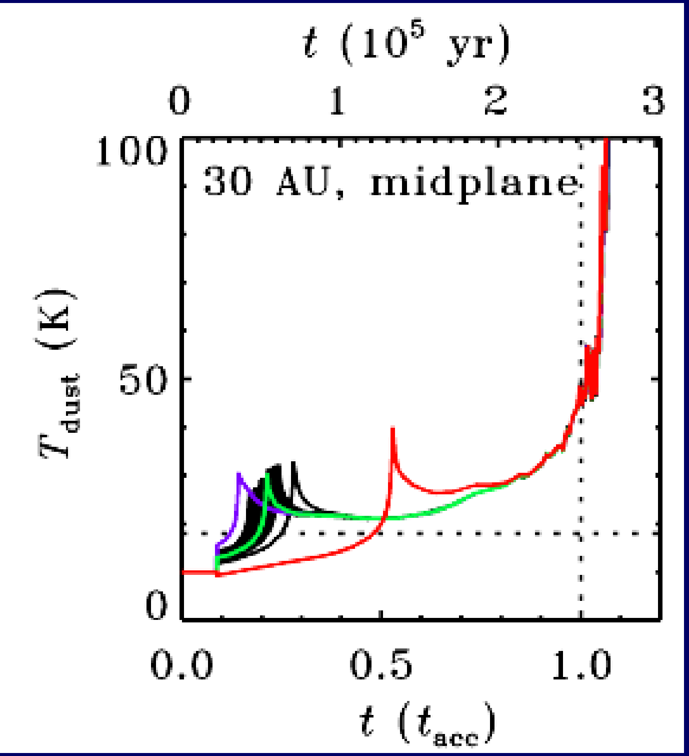
Changing initial conditions

- Lower sound speed:
  - Collapse time increases, luminosity decreases
  - Larger and colder disk
  - More ice
- Lower rotation rate:
  - More spherically symmetric, luminosity increases
  - Smaller and warmer disk
  - Less ice
- Lower initial mass:
  - Smaller and warmer disk
  - Less ice

Complex organics formation

(Garrod et al. 2006)

- First generation
  - Formed on grains
  - Need several 10^4 yr at 20–40 K
  - Possible in our model
- Second generation
  - Formed in warm gas (hot core)
  - Need several 10^3 yr at >100 K
  - Does not occur in our model



- Material in comet-forming zone (5–30 AU) probably abundant in complex organics
  - Spatial variations are likely

Future plans

- Full gas-phase network
- Mixed ices in more detail?
  - Need laboratory input
- Increase spatial resolution of the model
- Compute line profiles and compare with observations

Conclusions

- Gas/ice ratios change during collapse:
  - CO ice desorbs during infall, re-adsorbs in disk below 18 K
  - H_2O remains solid, except within a few AU
- Complex organics (first generation) abundant in planet-forming material
  - Spatial variation likely
- Only outer part of disk contains chemically pristine material
- Need mixed ices to explain CO in comets