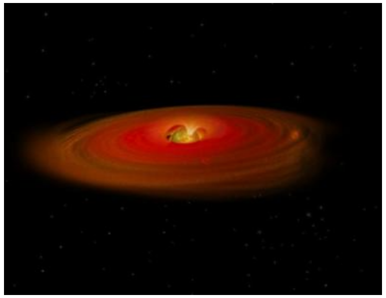
Chemical evolution from cores to disks



Ruud Visser
Leiden Observatory

Ewine van Dishoeck, Christian Brinch, Michiel Hogerheijde, Steve Doty, Kees Dullemond, John Black, Jes Jørgensen

September 21, 2009

Disks & chemistry: why do we care?

Circumstellar disks

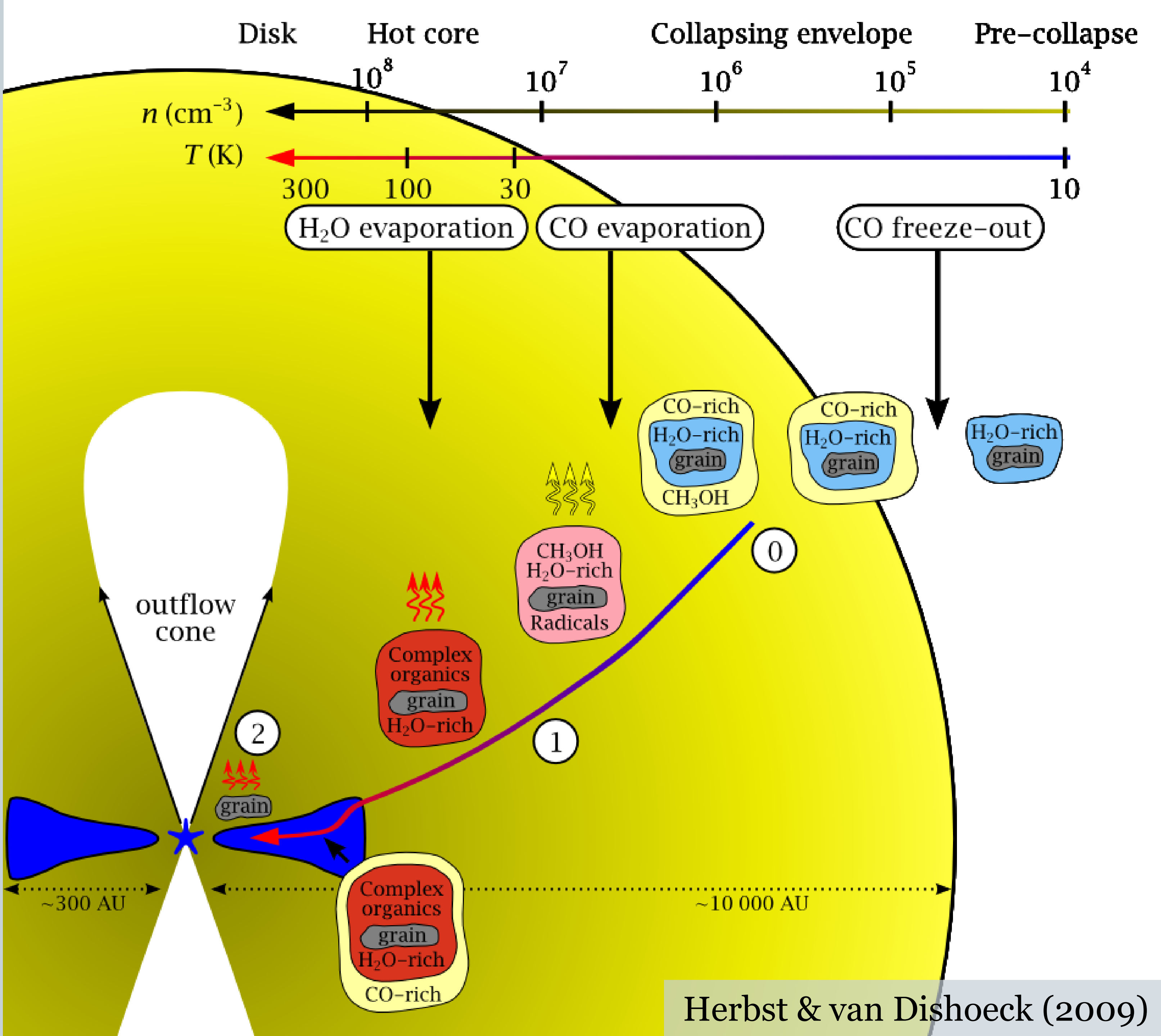
- Important aspect of star formation
- Formation site of planets and comets
- Indirect origin of interplanetary dust and zodiacal light

Chemistry

- Spectroscopic observations often target molecules
- Chemistry traces physical properties
- Chemical composition of solar nebula inherited by planets and comets

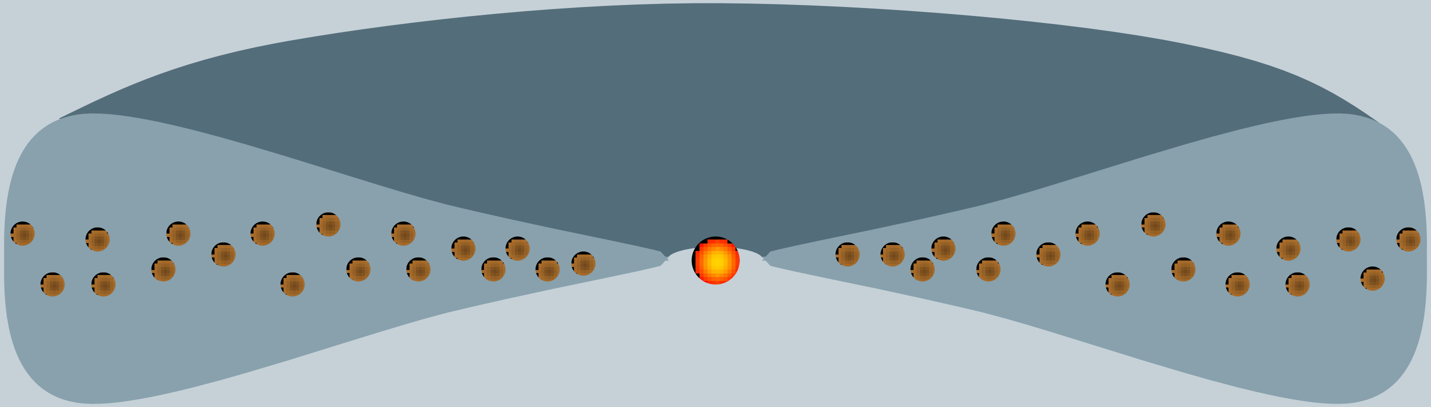
Low-mass star formation

Evolution of gas and dust



Herbst & van Dishoeck (2009)

T Tauri star and disk



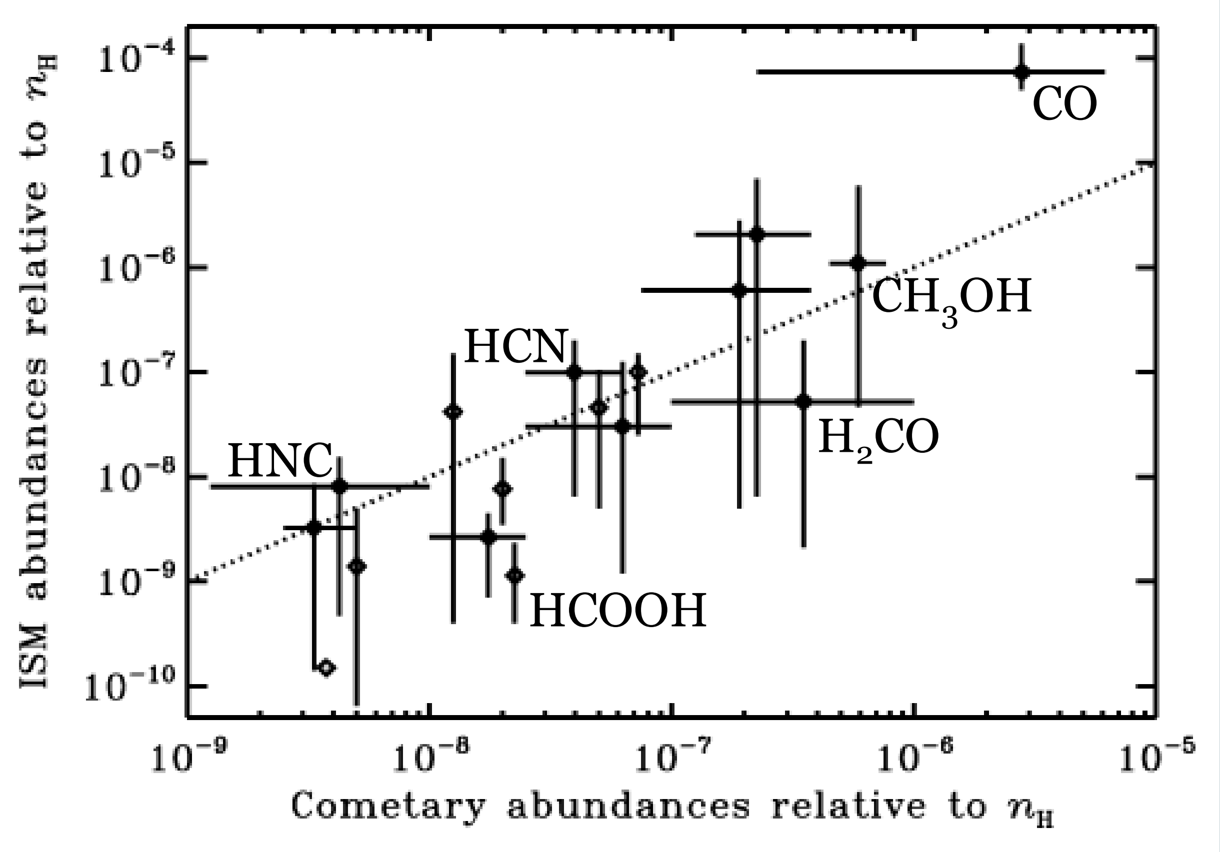
Star

- Low-mass: $< 2\ M_\odot$
- Age: few Myr

Disk

- Lifetime: ~10 Myr
- Size: few 100 AU
- Mass: $\sim 0.001\text{–}0.1\ M_\odot$
- Grains growth

Comets: a view of the past



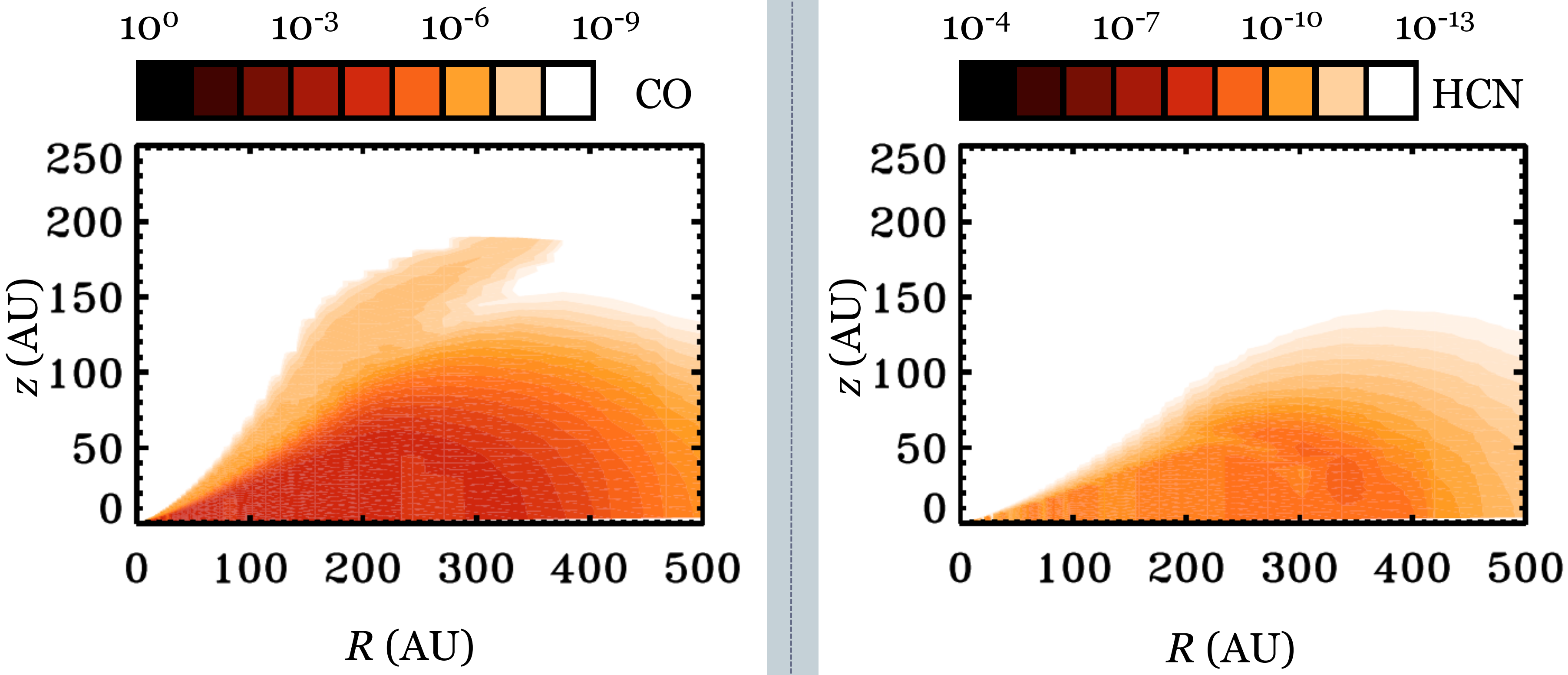
- Error bars indicate spread between sources
- Dotted line: hypothetical one-to-one relationship
- Comets in general similar to ISM, but individual differences exist

Bockelée-Morvan et al. (2000, 2004), Schöier et al. (2002)

Open questions

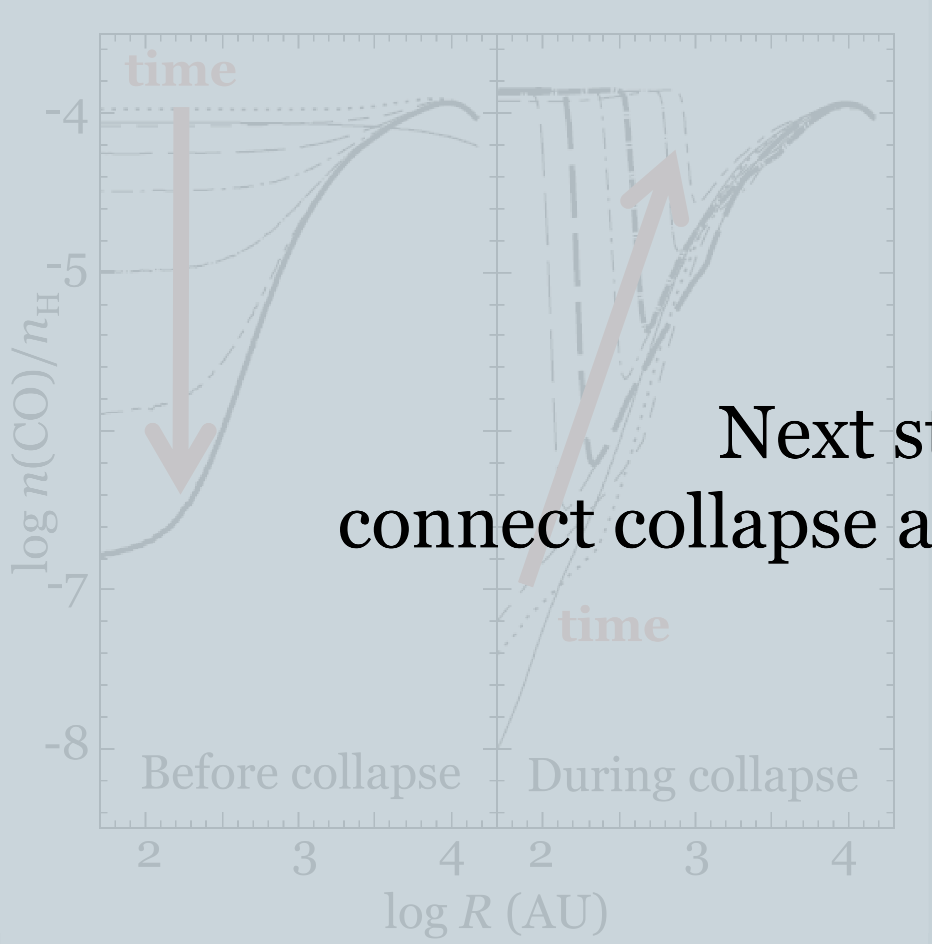
- Does material from the envelope accrete on the inner or outer parts of the disk?
- How does the chemical composition change from the envelope to the disk?
- Does the collapse-phase chemistry survive into the T Tauri stages or is it erased by in situ processing?
- What fraction of cometary ices is truly pristine?
- What is the origin of the chemical diversity of comets?

Chemistry in static disk models



Jonkheid et al. (2007)

Chemical evolution in 1D



- Freeze-out towards center before onset of collapse
- Warm-up during collapse leads to evaporation
- Abundances of many molecules controlled by CO gas abundance

Next step:
connect collapse and disk models

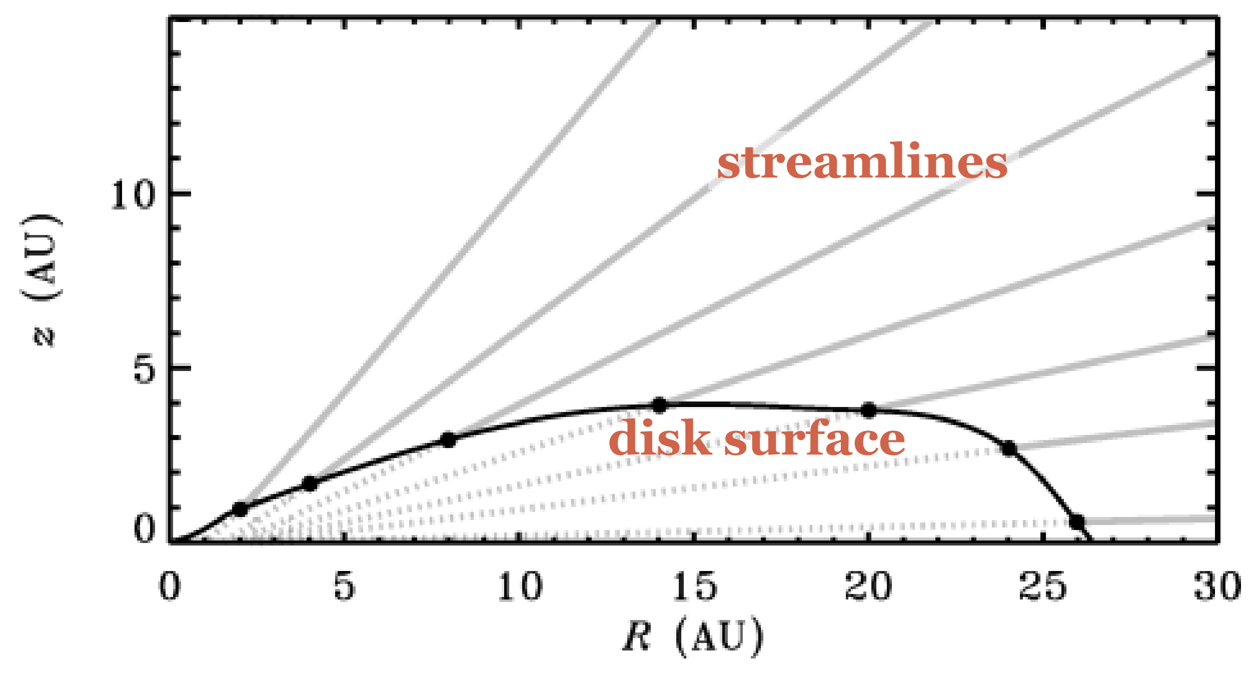
Lee, Bergin & Evans (2004)

Analytical star formation model in 2D

- Fast to run, high resolution,
  easy to change initial conditions
  Cloud mass, rotation rate, sound speed, ...
- 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 hydrodynamical models
  Yorke & Bodenheimer 1999, Brinch et al. 2008a,b
- Density profiles compare well with observations
  Jørgensen et al. 2009

Visser et al. (2009), Visser & Dullemond (in prep.)

From one to two dimensions

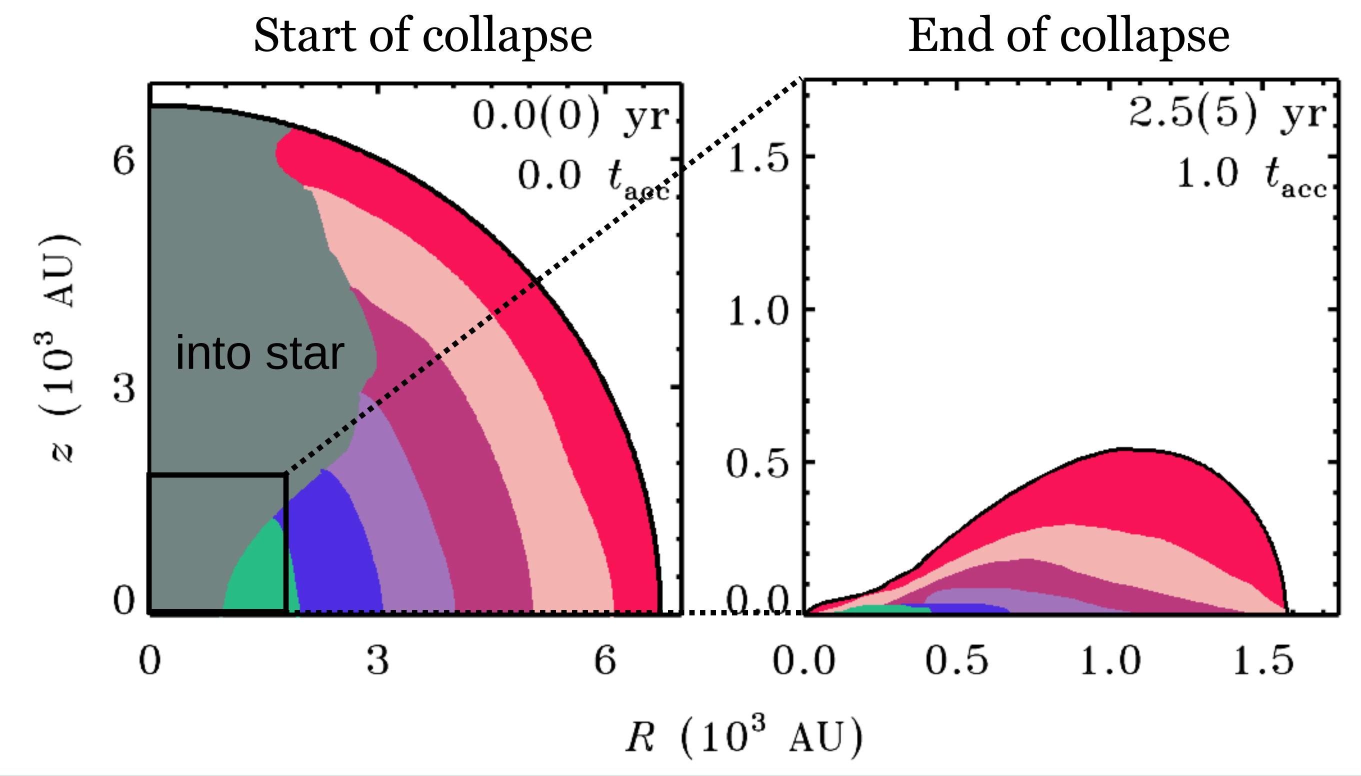


- Previous collapse models treated disk as completely flat
- Include vertical structure: accretion occurs further out

Visser & Dullemond (in prep.)

Where does material go to?

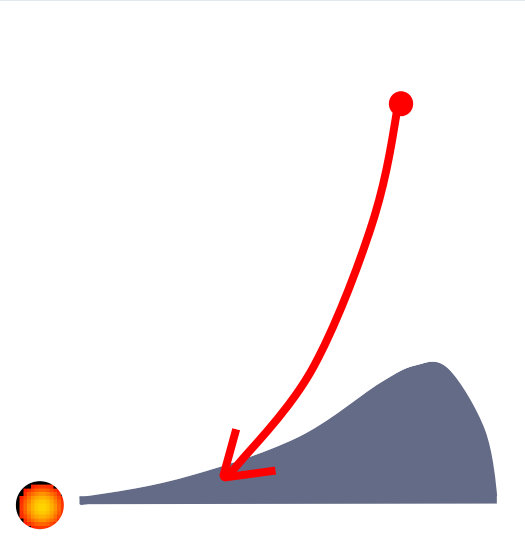
Inside-out collapse gives a layered disk

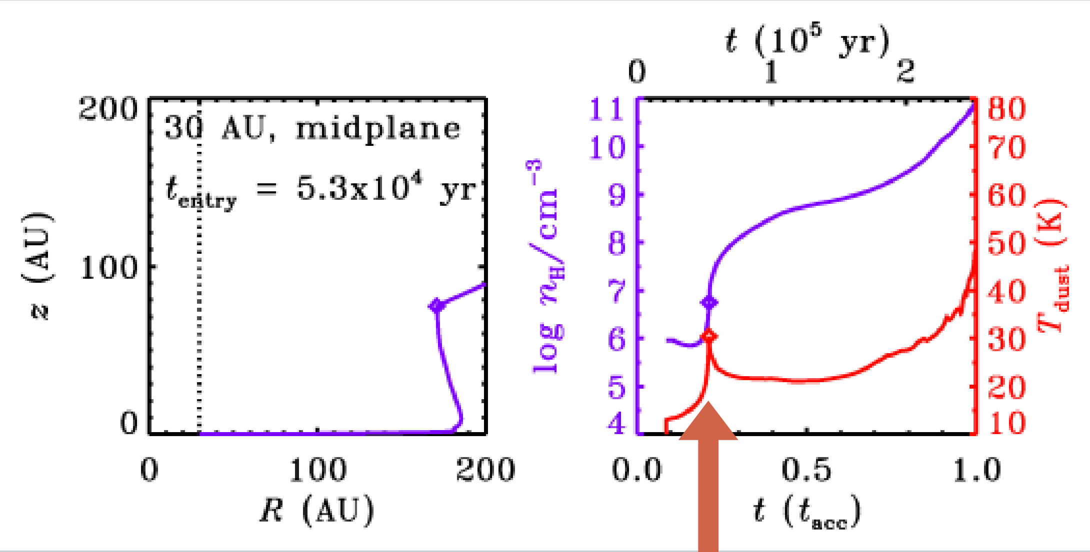


Visser et al. (2009)

Infalling trajectories

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



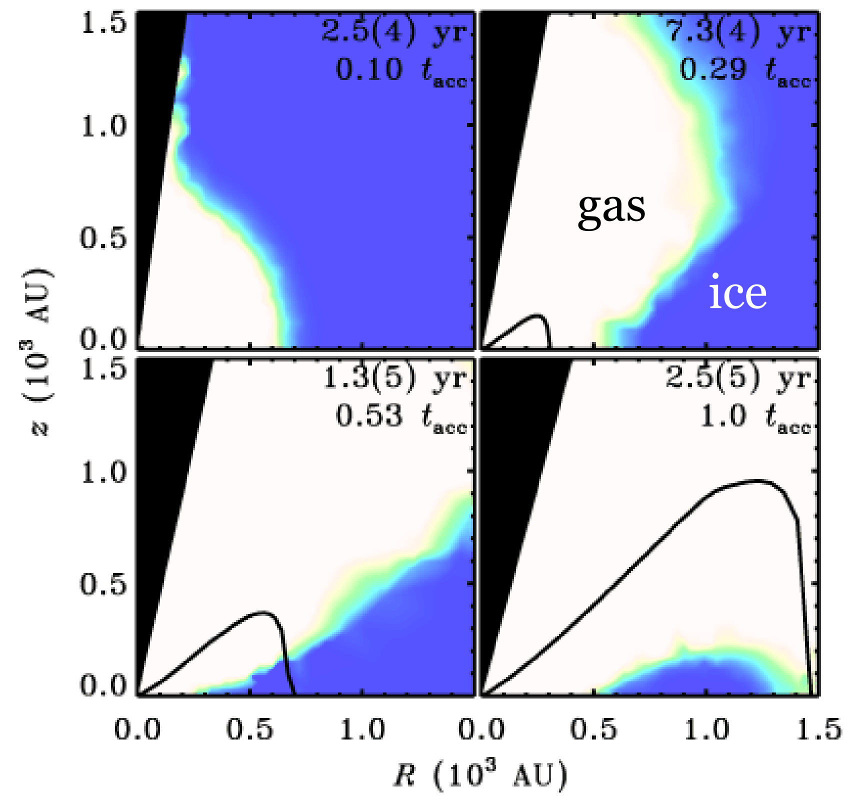


- Jump in n, T upon entering disk
- n increases by factor of ~10^5 overall, T goes from 10 to several 10s of K

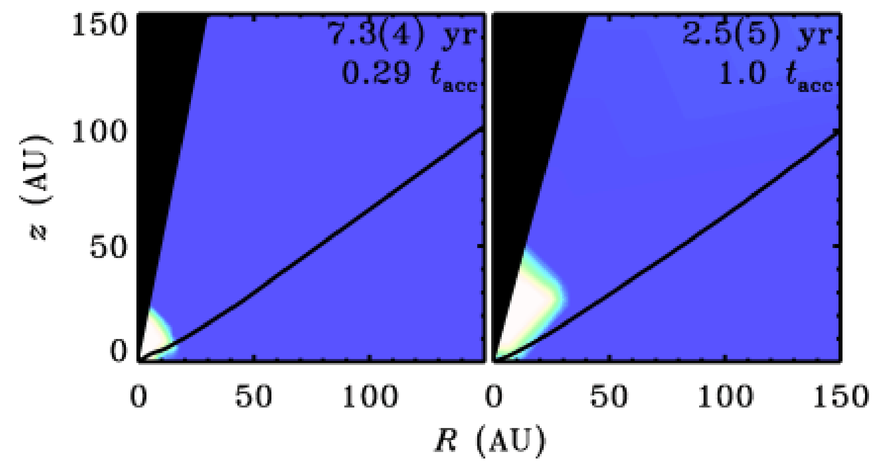
entering disk

Visser et al. (2009)

First test: gas and ice



CO



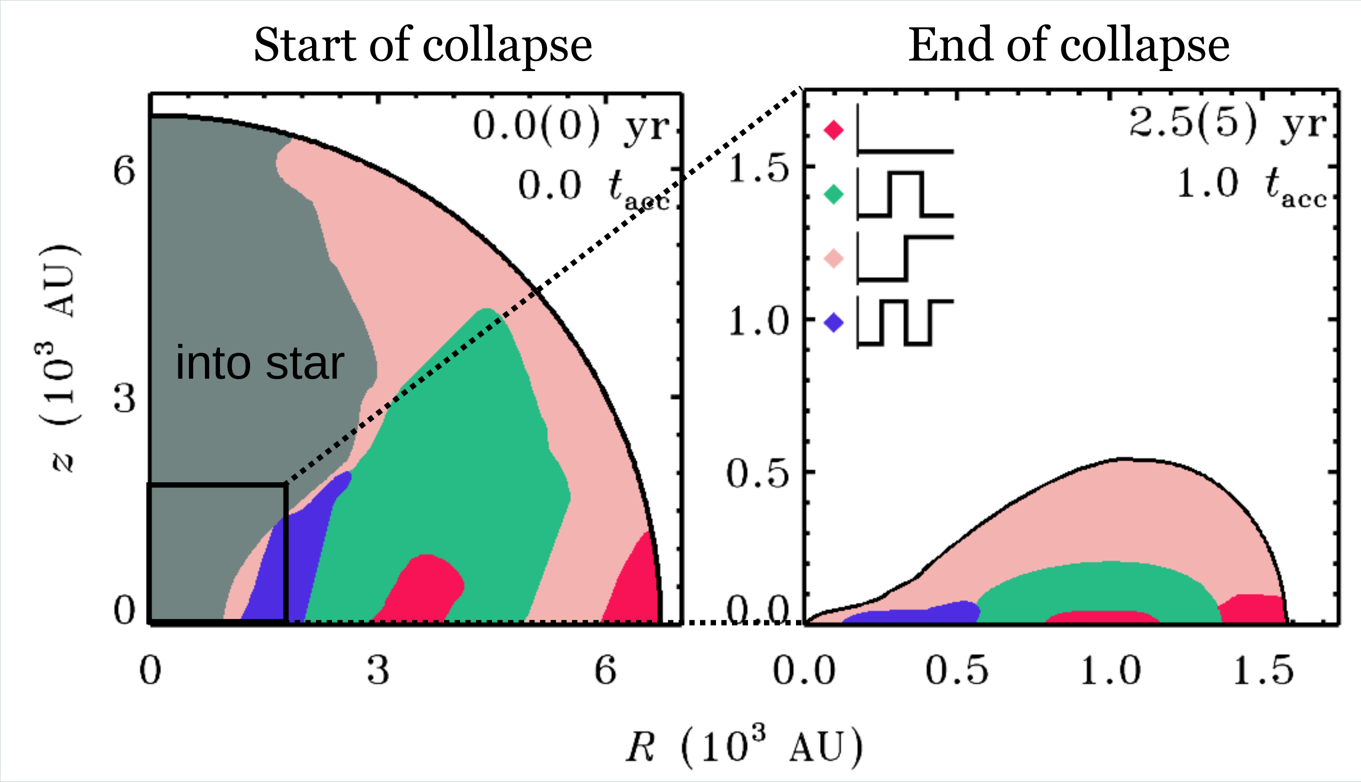
H_2O

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

Visser et al. (2009)

Chemical zones: CO gas/ice



Red: CO remains adsorbed (pristine!)

Green: CO desorbs and re-adsorbs

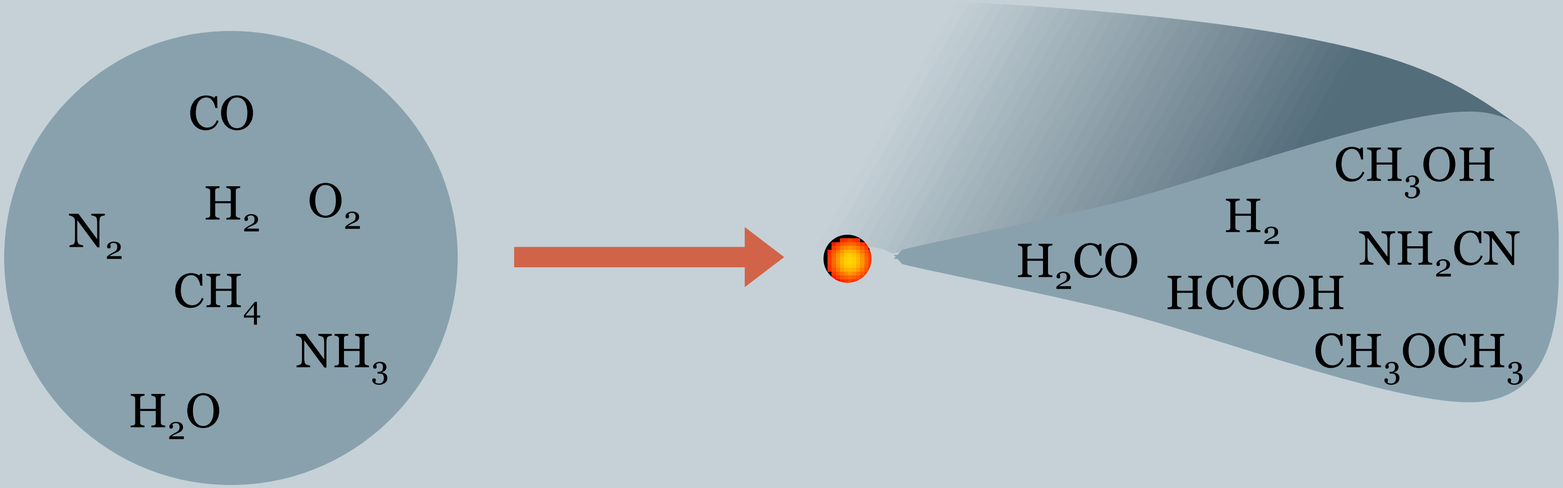
Pink: CO desorbs and remains desorbed

Blue: multiple desorption/adsorption

Visser et al. (2009)

Full chemical model

- ~450 molecules connected by ~4500 reactions
- Reaction rates depend on n_H, T, F_UV, A_V
- Start with simple composition
- Follow abundances along infall trajectories



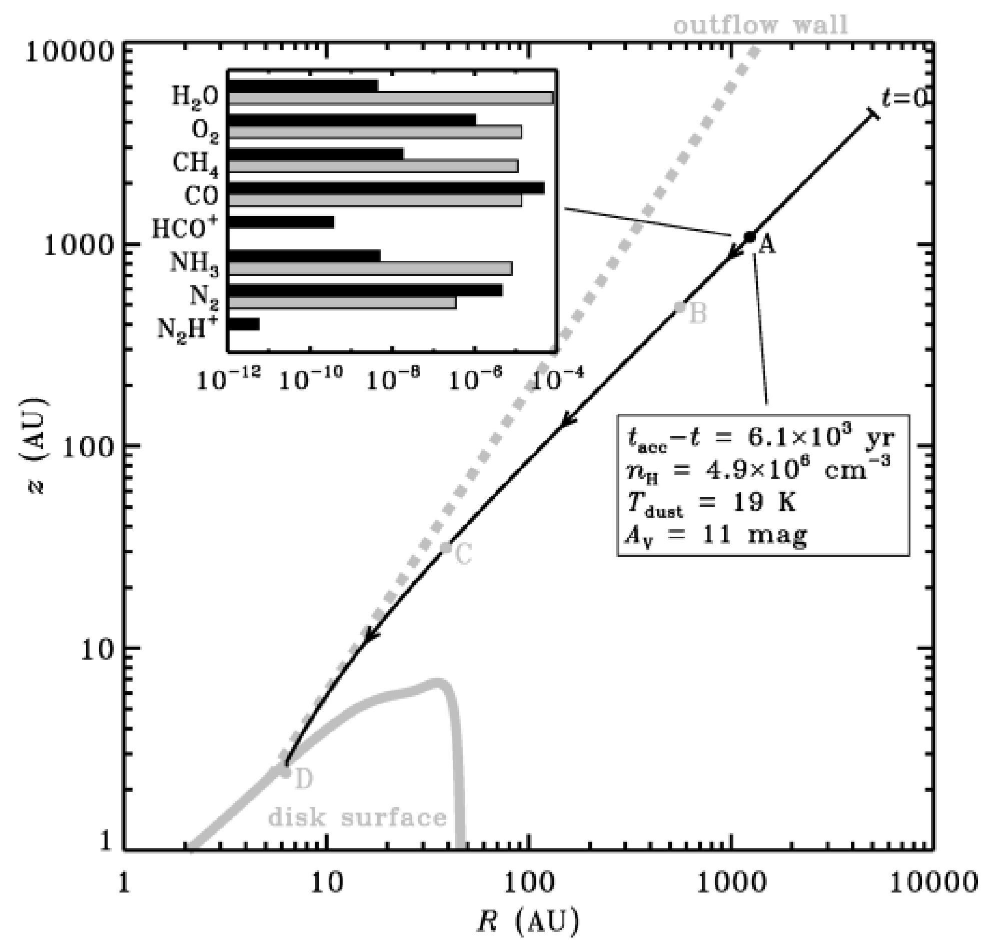
Visser et al. (in prep.)

Chemical evolution along one trajectory

- Initial composition: atomic except H_2
- Keep static for 1 Myr
- At onset of collapse:
  - Oxygen mainly in H_2O ice, CO ice, O_2 ice
  - Carbon mainly in CO ice, CH_4 ice
  - Nitrogen mainly in N_2 ice, NH3 ice, NO ice

Visser et al. (in prep.)

Chemical evolution along one trajectory

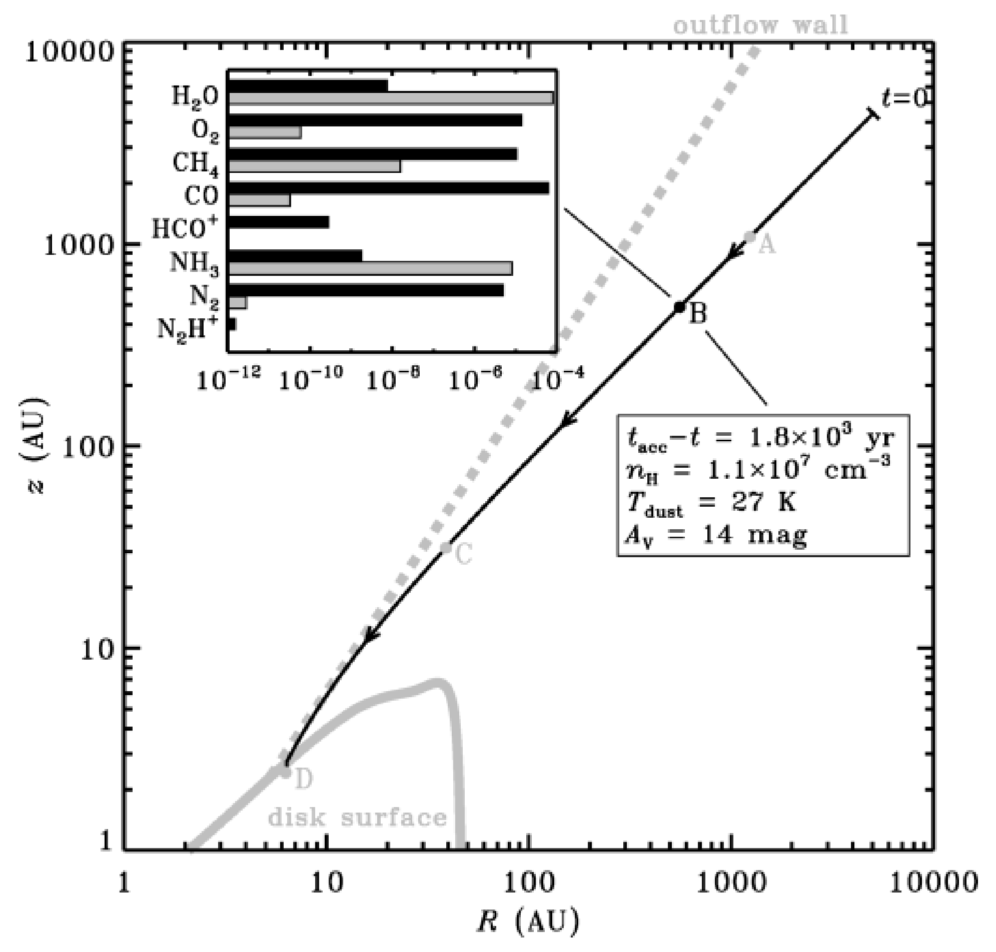


Point A:

- CO, N_2, O_2 evaporate
- HCO^+, N_2H^+ formed
- H_2O, CH_4, NH_3, NO remain frozen

Visser et al. (in prep.)

Chemical evolution along one trajectory

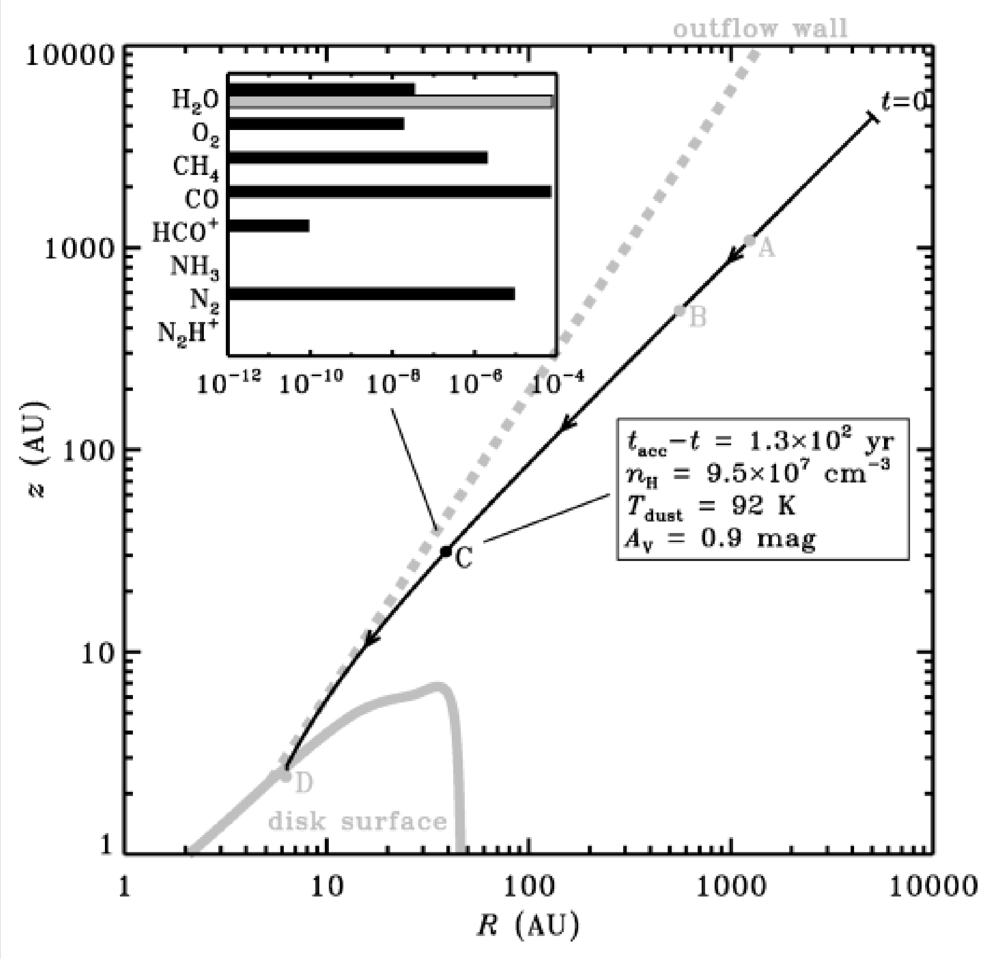


Point B:

- CH_4, NO evaporate
- CO, N_2, O_2 remain in gas
- H_2O, NH_3 remain frozen

Visser et al. (in prep.)

Chemical evolution along one trajectory

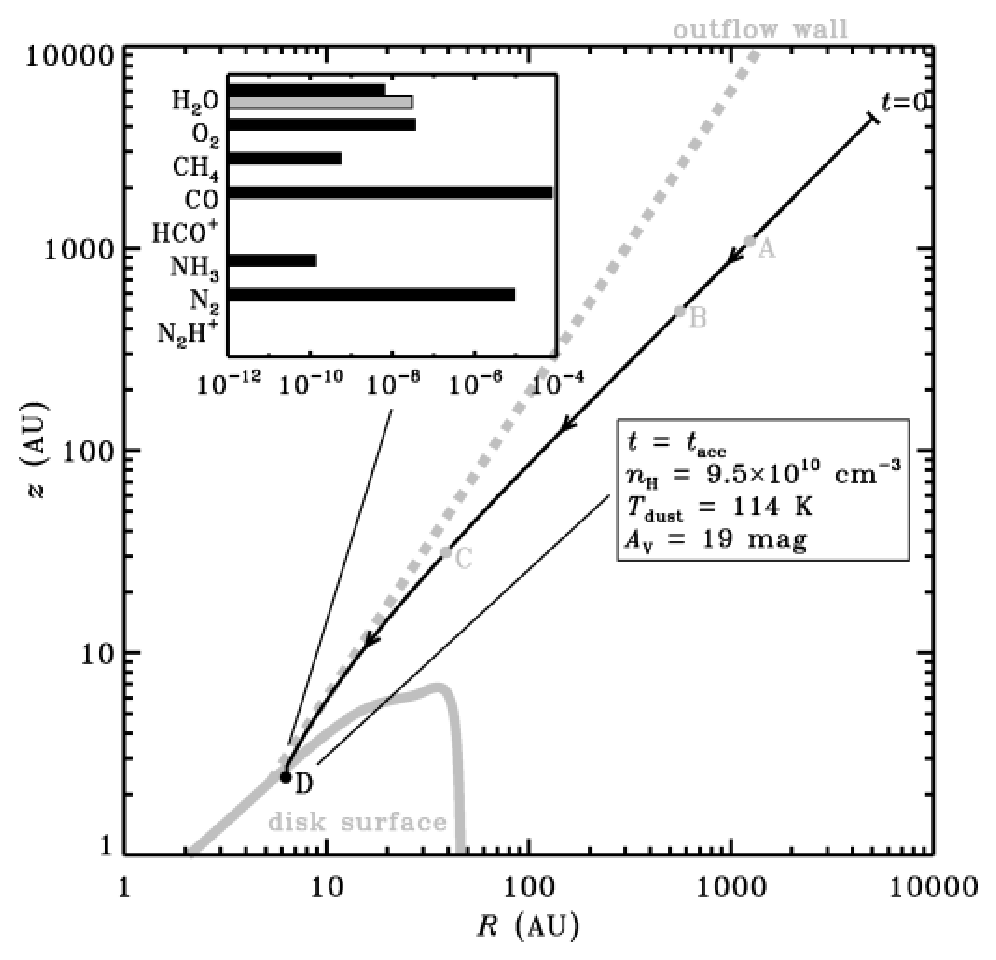


Point C:

- NH_3, H_2O evaporate
- NH_3, H_2O, O_2, CH_4 are photodissociated
- CO, N_2 survive

Visser et al. (in prep.)

Chemical evolution along one trajectory

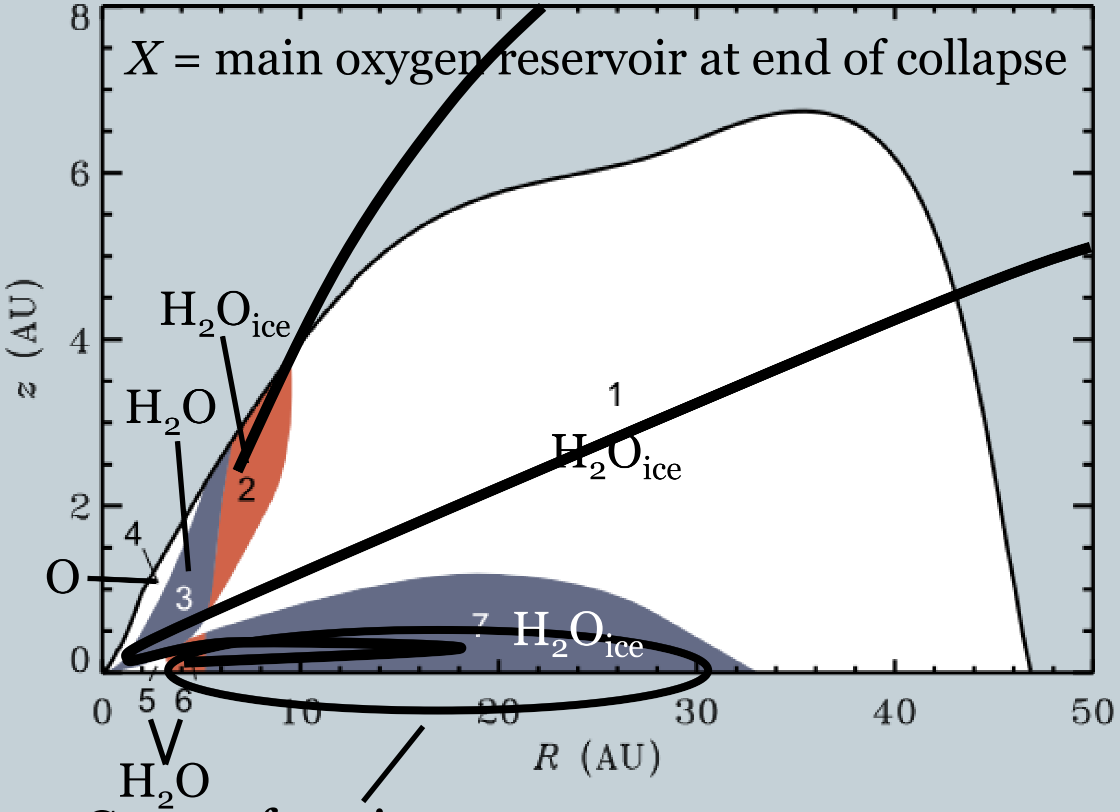


Point D:

- Some NH_3, H_2O, CH_4 reformed
- CO, N_2 most abundant

Visser et al. (in prep.)

Water zones

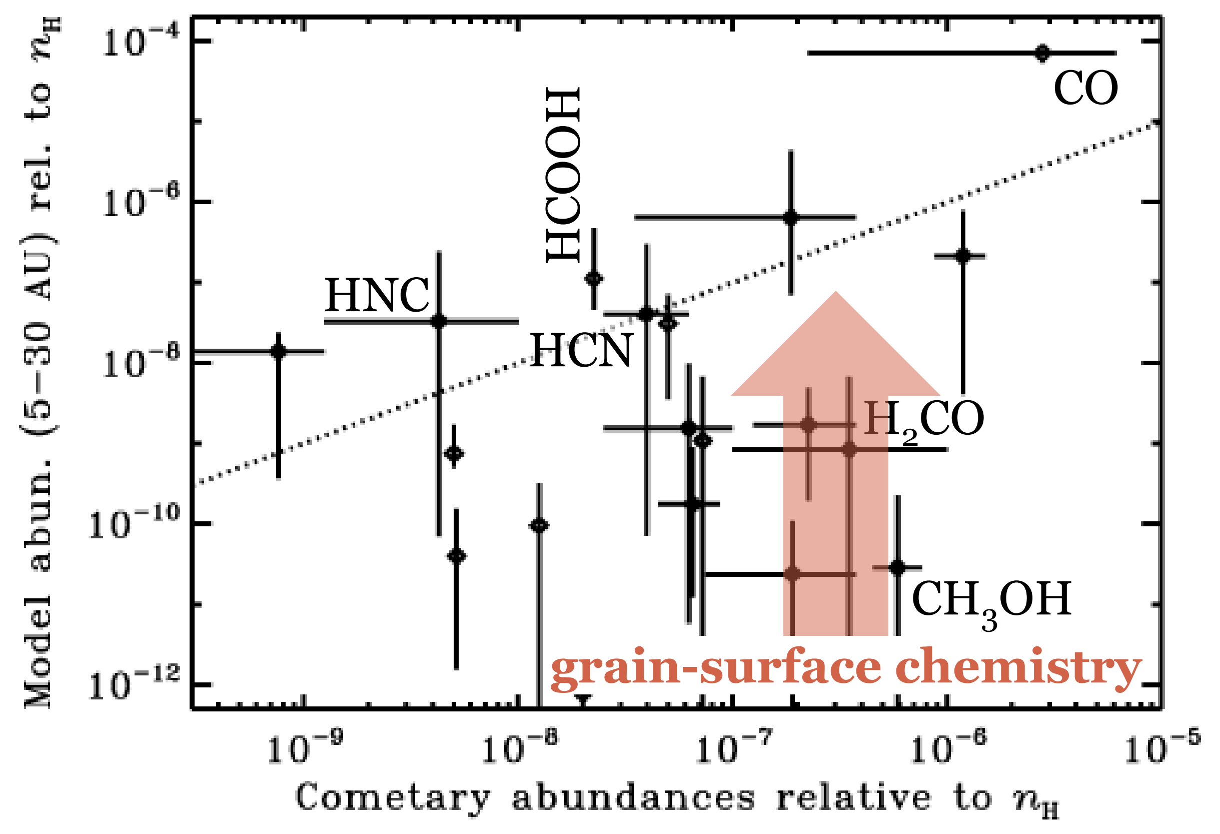


Comet-forming zone

1. Always frozen
2. Evaporates, photodissociated, reformed, freezes out
3. Evaporates, photodissociated, reformed
4. Evaporates, photodissociated
5. Evaporates
6. Evaporates, freezes out, evaporates
7. Evaporates, freezes out

Visser et al. (in prep.)

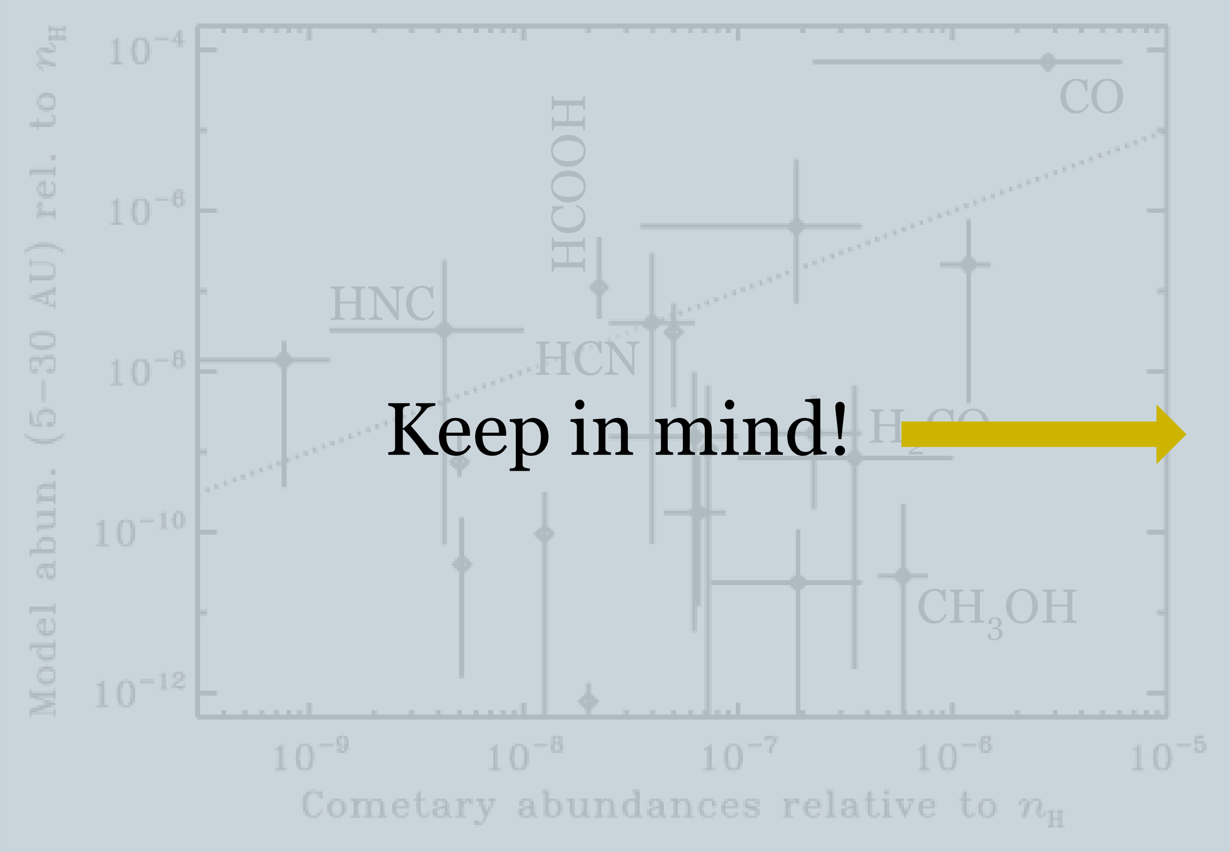
Implications for comets



- Dotted line: hypothetical one-to-one relationship
- Many model abundances differ from cometary abundances
- Suggestive of mixing or grain-surface chemistry?

Visser et al. (in prep.)

Implications for comets



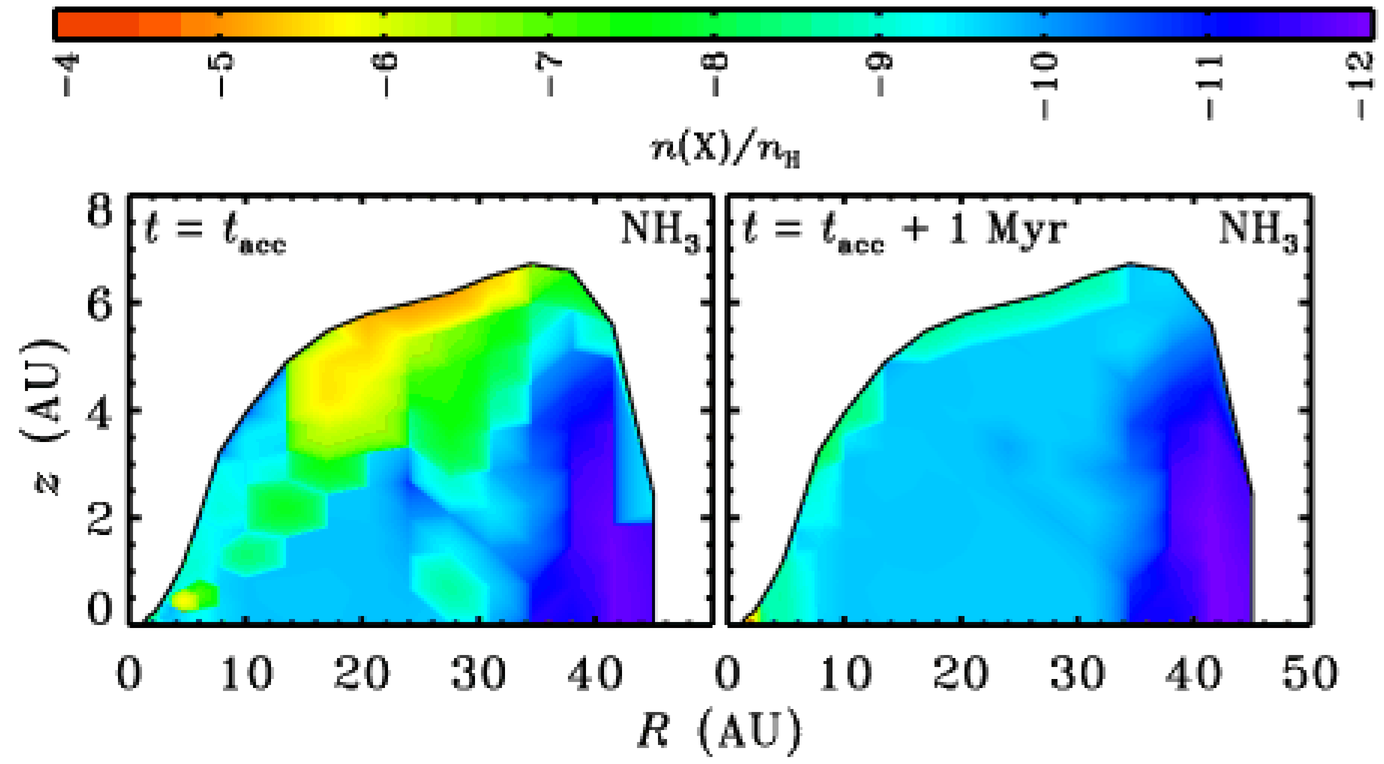
Keep in mind!

- Dotted line: hypothetical one-to-one relationship
- Many model abundances differ from cometary abundances
- Suggestive of mixing or grain-surface chemistry?

Visser et al. (in prep.)

Collapse phase versus local processing

Simple test shows chemistry not in equilibrium at end of collapse



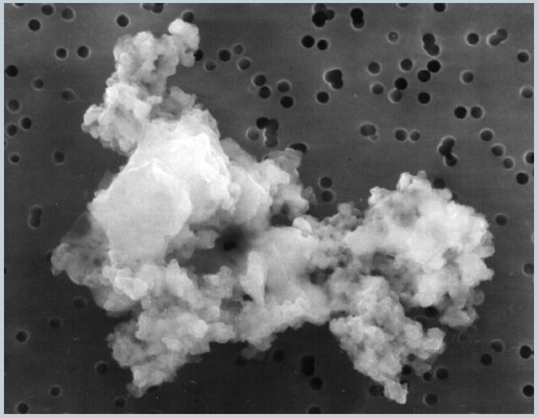
Visser et al. (in prep.)

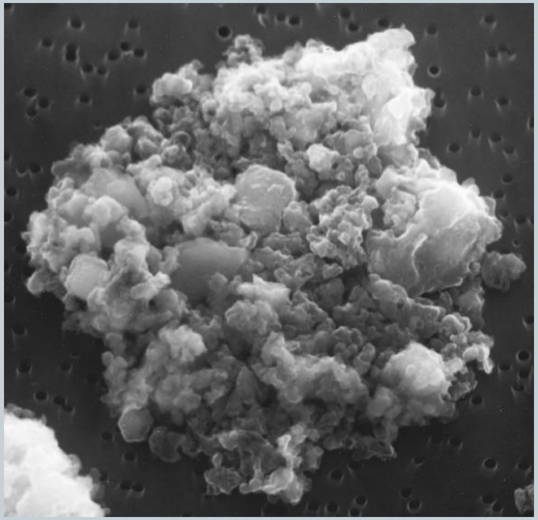
Summary so far

- Material accretes mostly on outer parts of disk
- Disk is divided into zones with different chemical histories
  - Outer part pristine, inner part processed
- Collapse-phase chemistry survives into T Tauri stage
- Composition of comet-forming zone matches poorly with composition of comets
- Chemical diversity of comets due to different formation positions or times

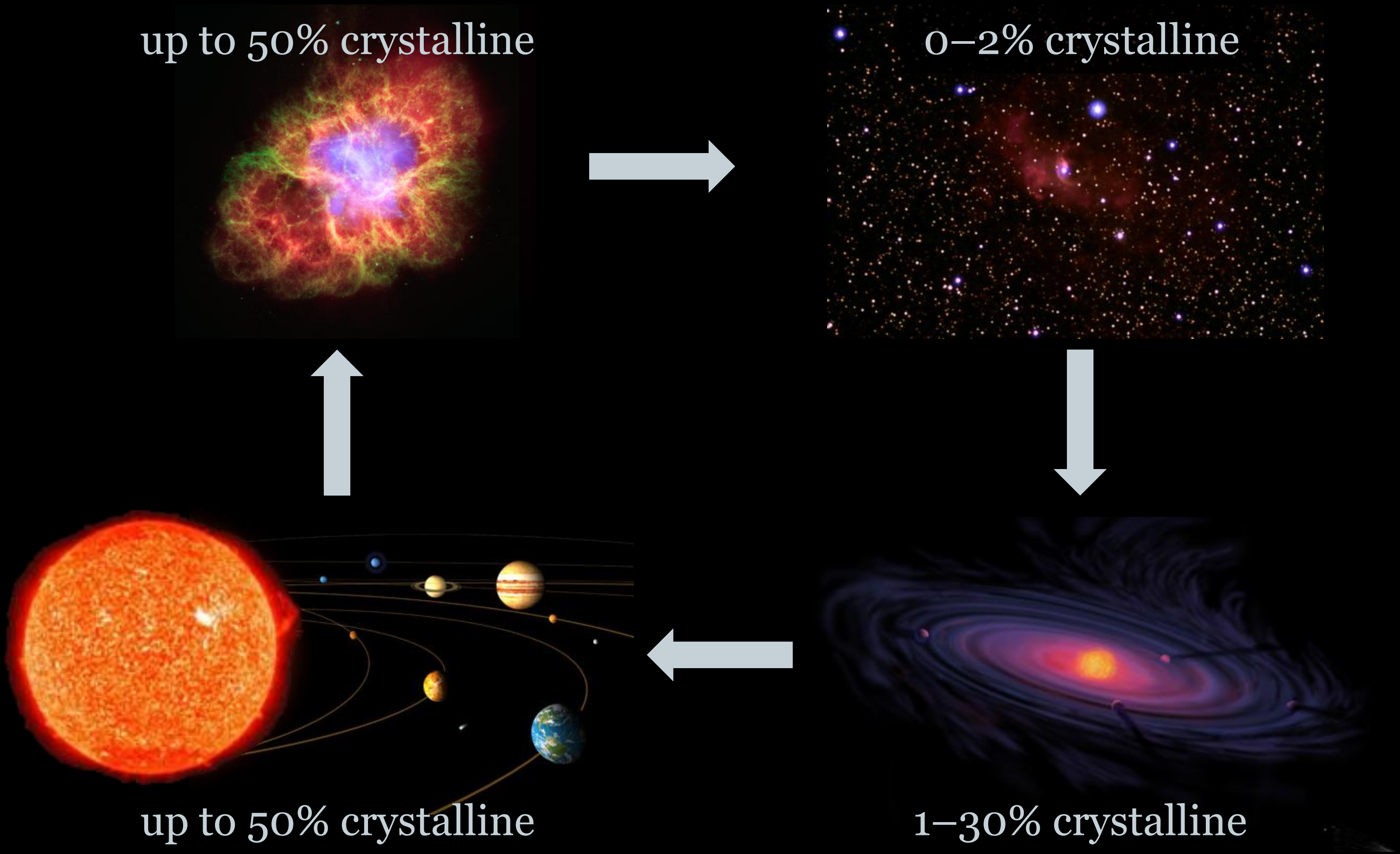
Another application of our model: dust

- Carbonaceous material
  - Graphite (small-scale limit: PAHs)
  - Hydrogenated amorphous carbon
  - Diamonds
- Silicates
  - Amorphous (olivine, pyroxene, …)
  - Crystalline (forsterite, enstatite, …)
- Ices
  - H_2O, CO, CO_2, CH_3OH, NH_3, …





From crystalline to amorphous and back



up to 50% crystalline

0–2% crystalline

1–30% crystalline

up to 50% crystalline

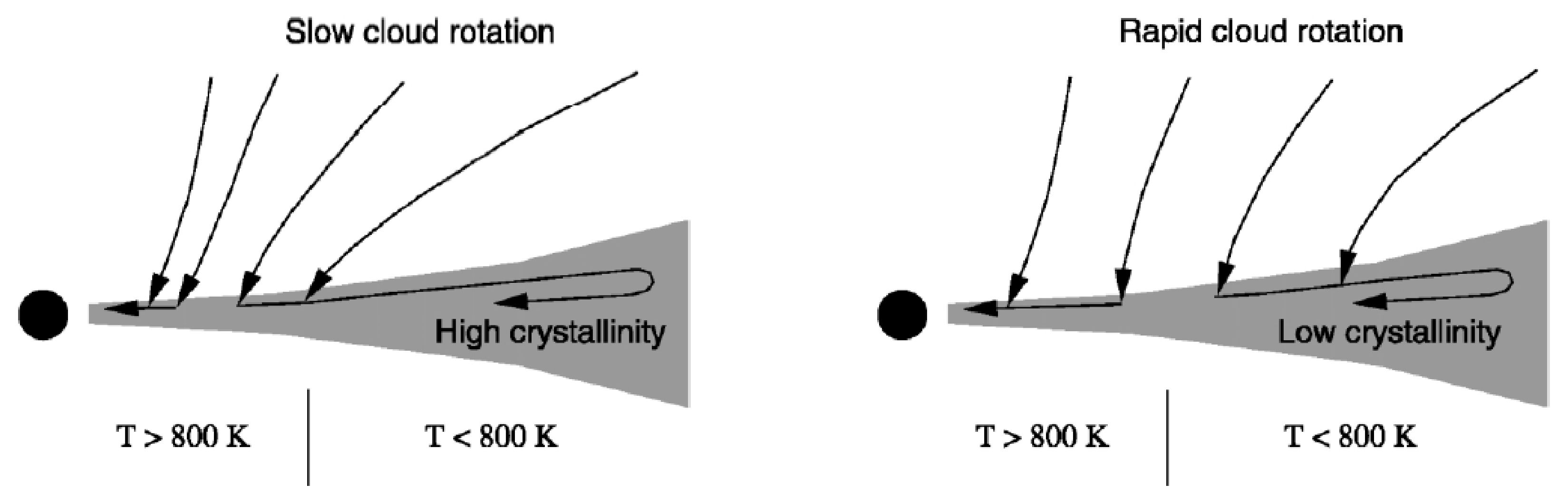
Dust processing

- ISM: 1% crystalline; disks: 1–30% crystalline
- Crystallization by thermal annealing requires 800 K
  - Works for material accreting close to the star
- Crystalline silicates observed down to 150 K and in comets formed in 100–200 K regions

How can we explain these cold crystalline silicates?

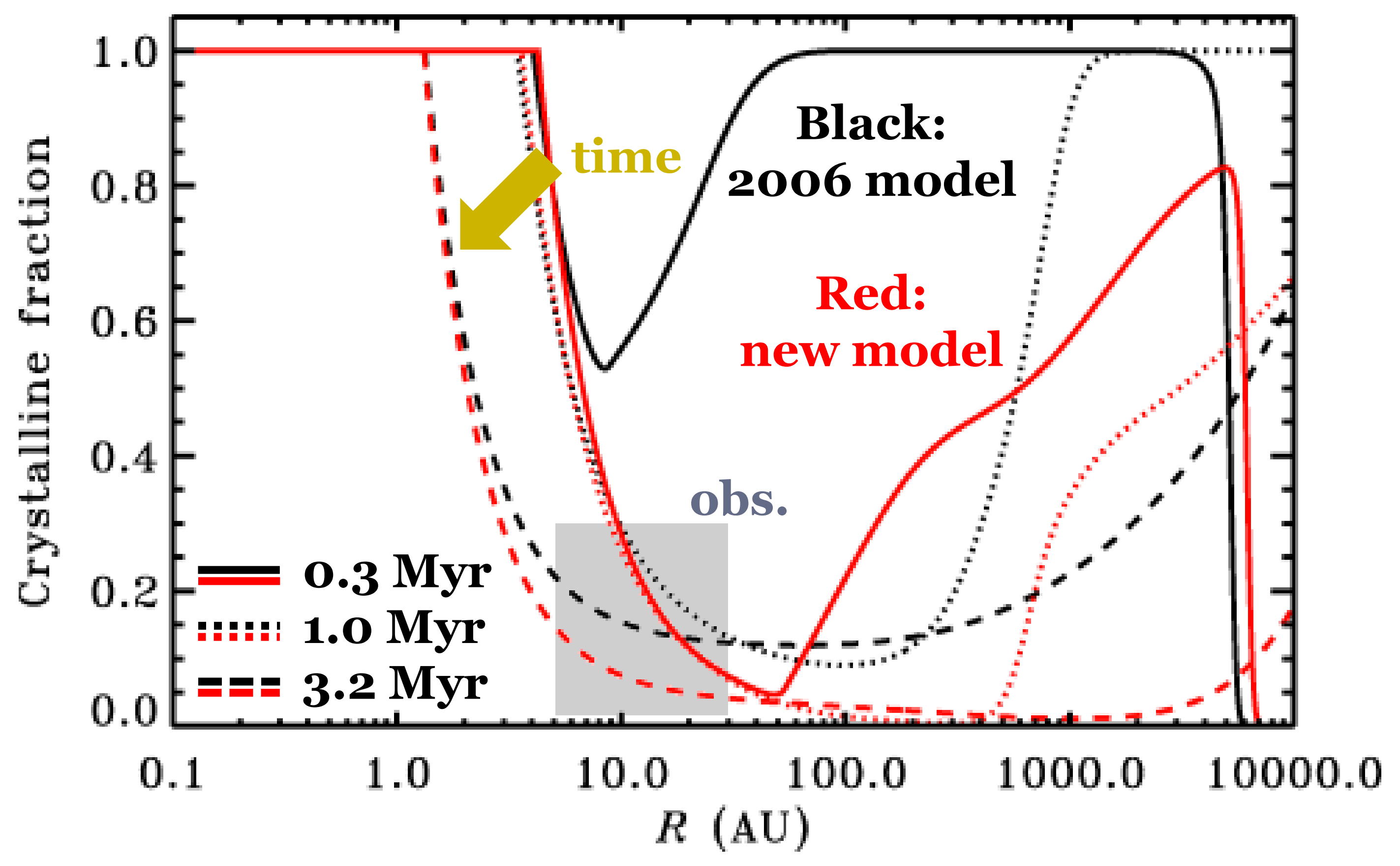
Disk evolution model

- Inside-out collapse with rotation
- Dust accreting in hot inner region is crystallized
- Disk spreads out to conserve angular momentum
- Crystalline material transported to colder areas



Dullemond, Apai & Walch (2006), Visser & Dullemond (in prep.)

Crystalline fractions



Model results in good agreement with observed range!

Visser & Dullemond (in prep.)

Implications for comets

Observations	Model
• Silicate dust	• Silicate dust
○ Partially crystalline	○ Partially crystalline
○ Partially amorphous	○ Partially amorphous
• Chemical composition	• Chemical composition
○ Generally similar to ISM	○ Outer disk unprocessed
○ Individual differences	○ Inner disk processed

Cometary material is of mixed origins

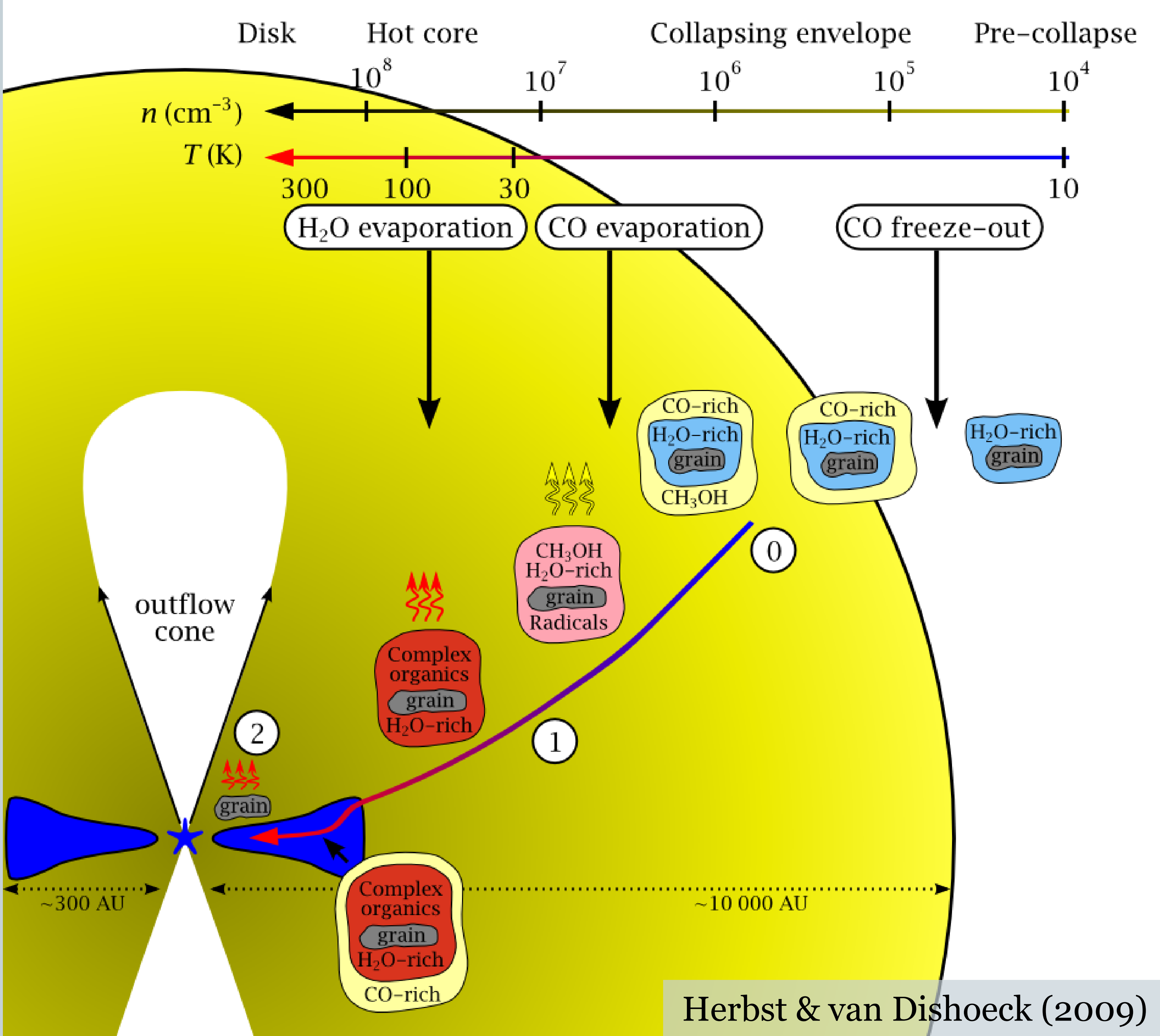
Caveats

- Gas temperature
  - Gas-phase production of water
  - Increase inner-disk scale height
- Shape of stellar spectrum
  - Allow photodissociation of H_2, CO, N_2
- Trapping of volatiles in water ice
  - Increase ice abundances of CO, N_2, O_2, …
- Mixing
  - Chemical zones in disk more diffuse

Future work

- Run chemistry for more parcels
  - ○ Increase spatial resolution
- Compute line profiles
  - ○ Compare with observations by JCMT, IRAM 30m, …
  - ○ Make predictions for Herschel, ALMA
- Investigate effect of outflow
  - ○ How much material is swept up?
- Add grain-surface chemistry
  - ○ Formation of complex organics
- Treat CO photodissociation in more detail
  - ○ New model: Visser, van Dishoeck & Black (2009)

Low-mass star formation



Herbst & van Dishoeck (2009)

Evolution of gas and dust

Conclusions

- Important to do collapse and disk formation in 2D
- Material accretes mostly on outer parts of disk
- Disk is divided into zones with different chemical histories
    - Outer part pristine, inner part processed
- Collapse-phase chemistry survives into T Tauri stage
- Cometary material is of mixed origins