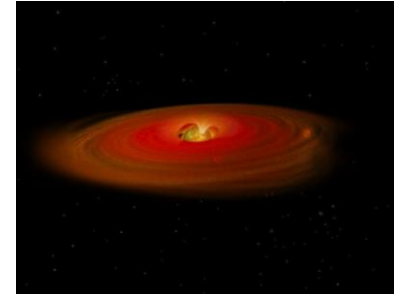




Chemical evolution from cores to disks



Ruud Visser
Leiden Observatory

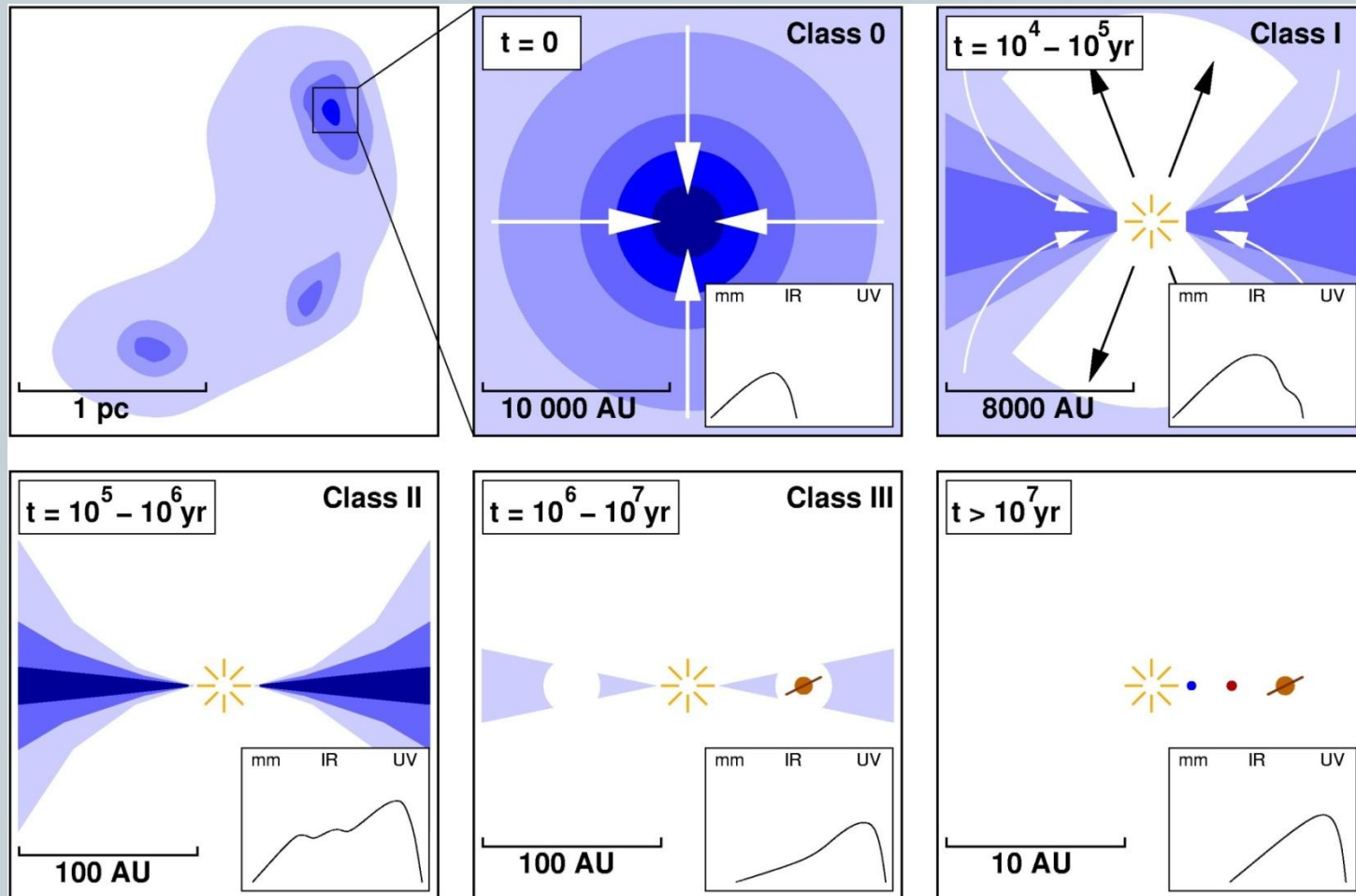
**Ewine van Dishoeck, Steve Doty, Kees
Dullemond, Jes Jørgensen, Christian
Brinch, Michiel Hogerheijde, John Black**



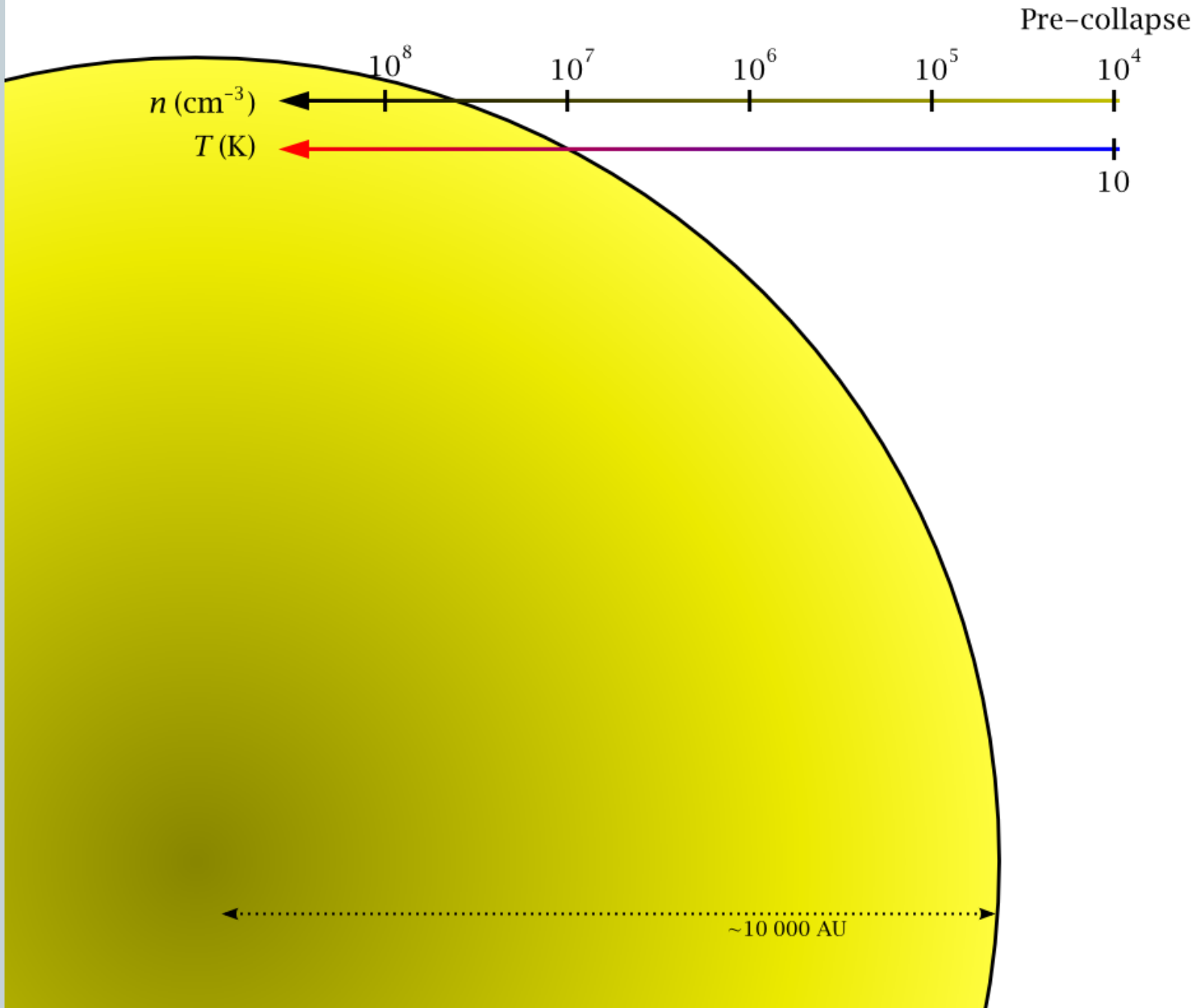
November 16, 2009



Low-mass star formation



Low-mass star formation

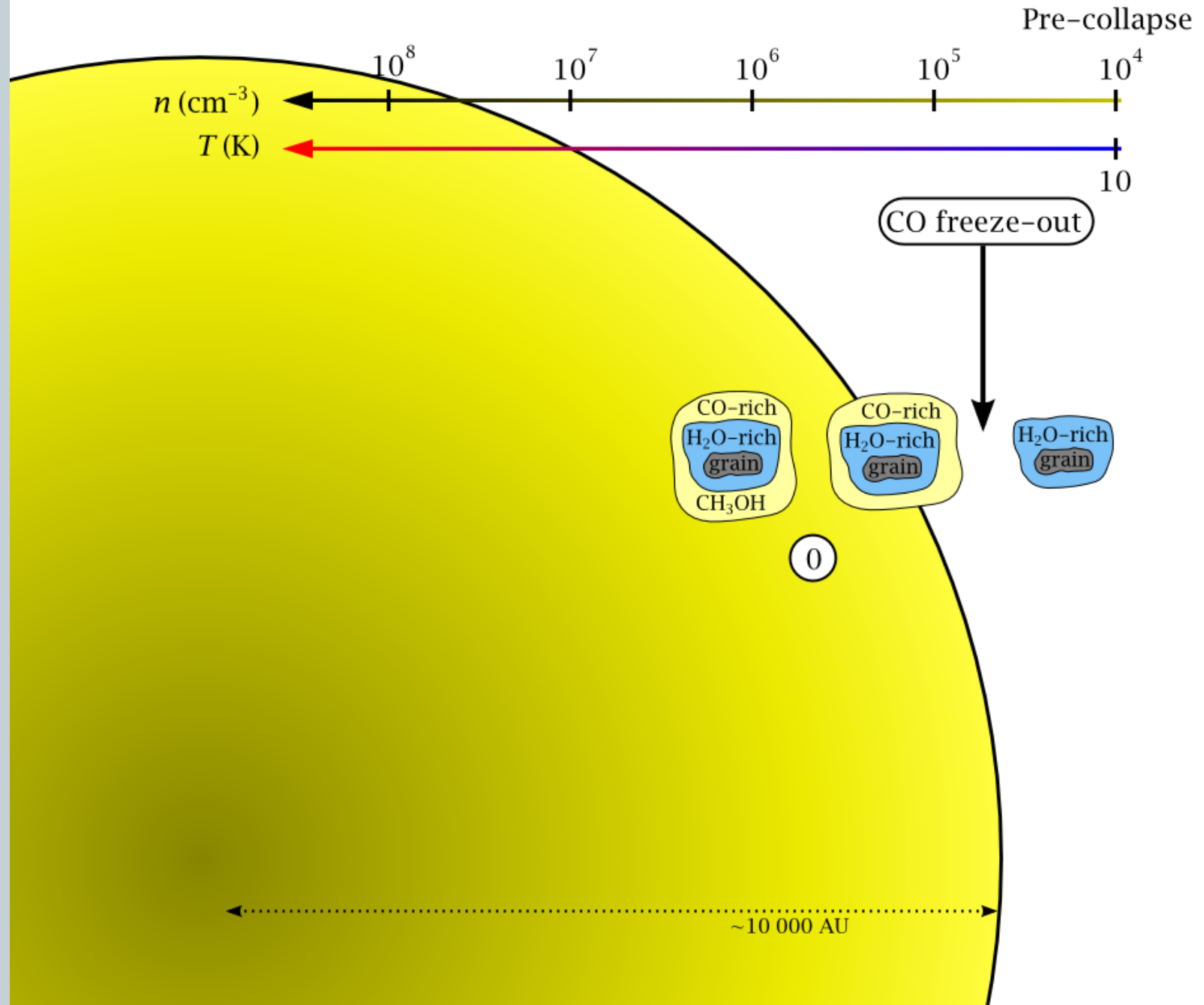


Evolution of gas and dust

Herbst & van Dishoeck (2009)

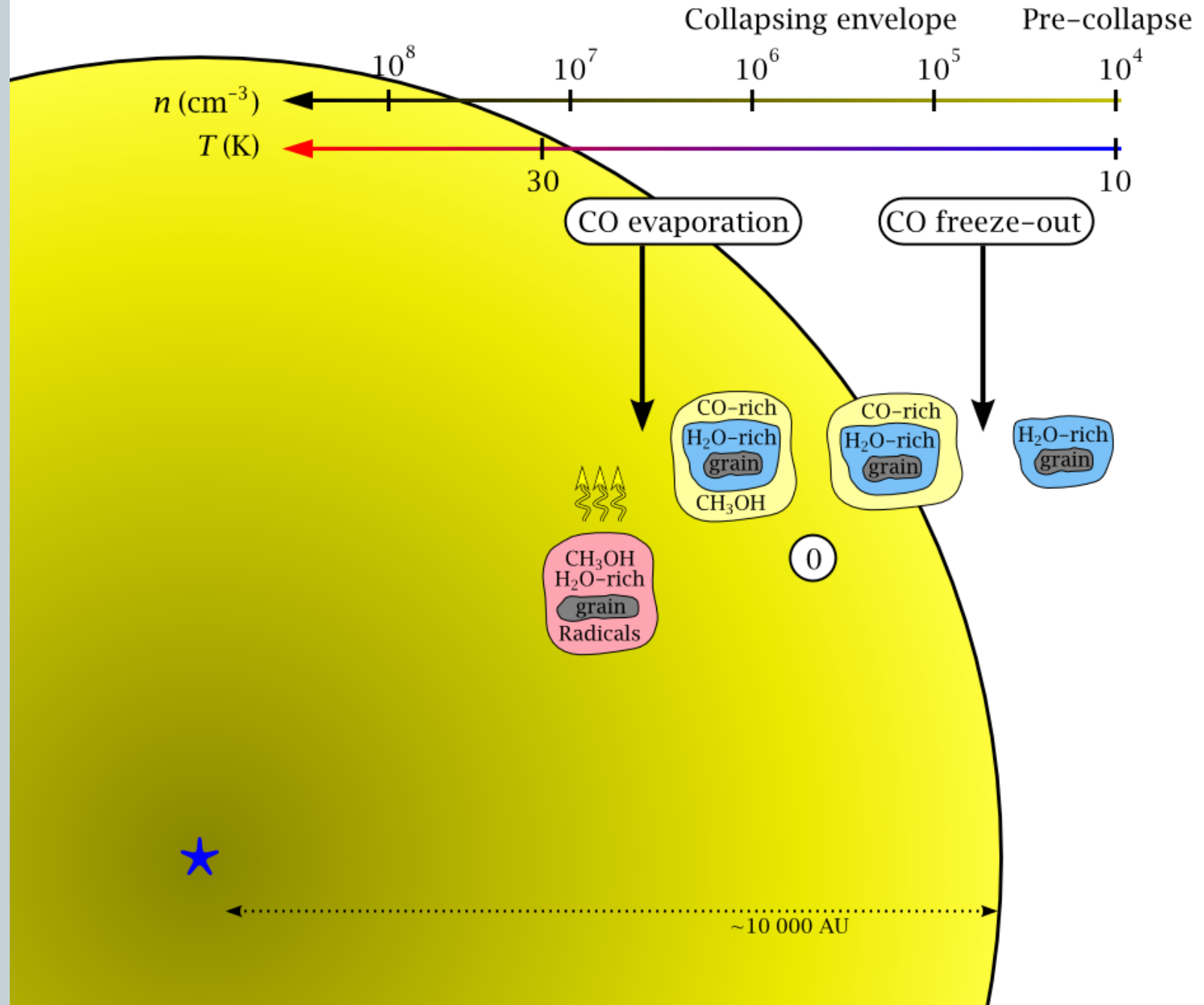
Low-mass star formation

Evolution of gas and dust



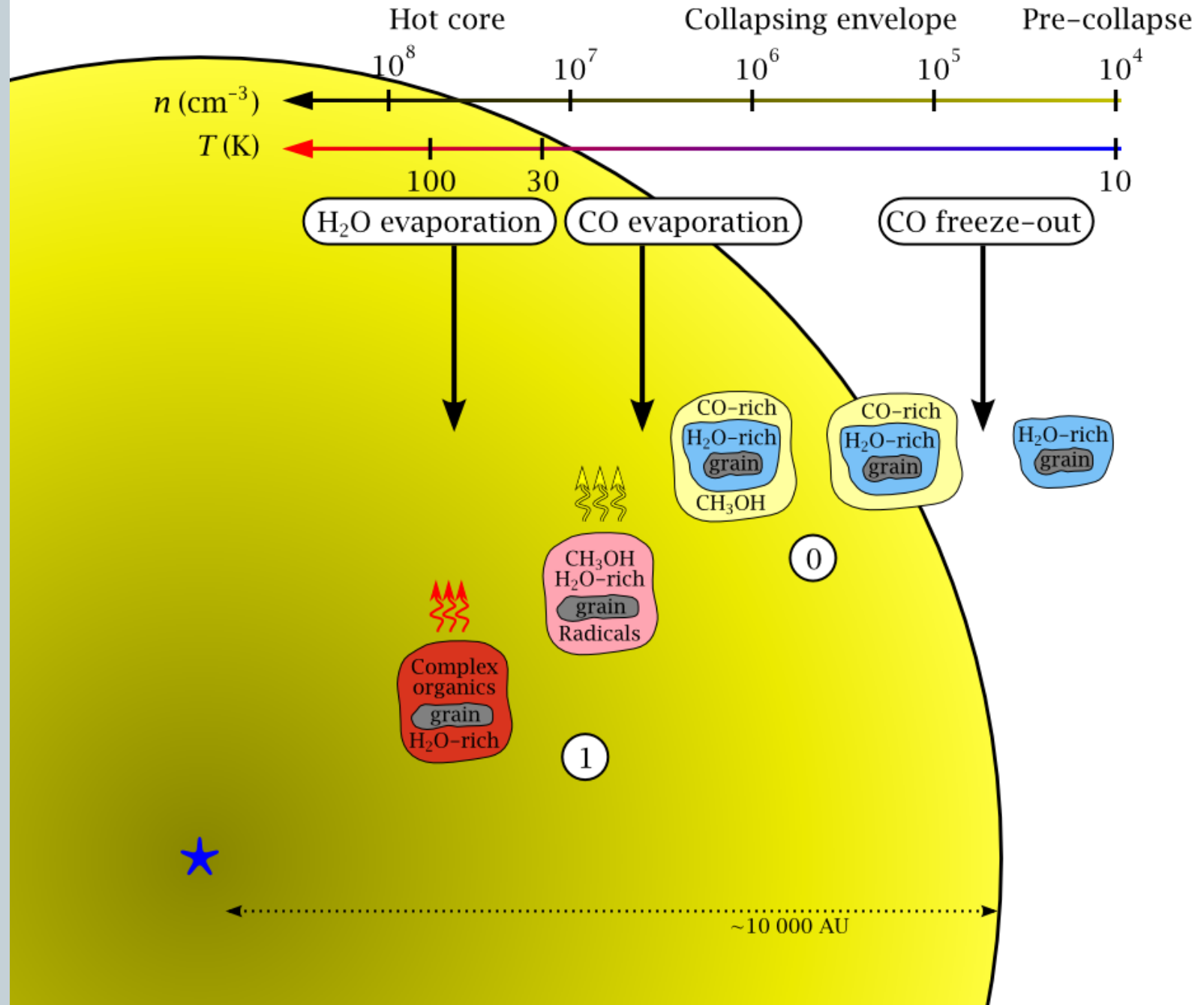
Low-mass star formation

Evolution of gas and dust

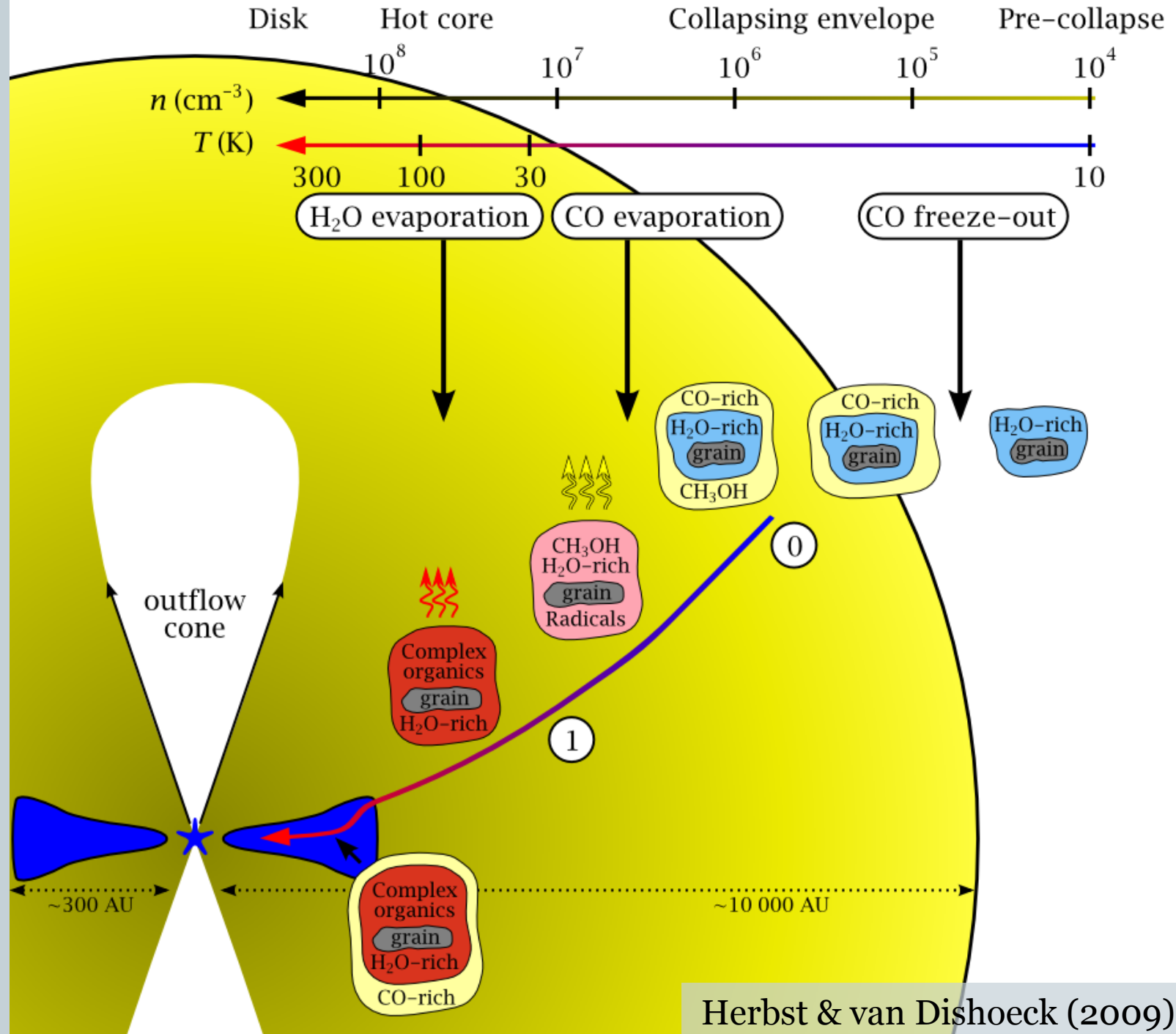


Low-mass star formation

Evolution of gas and dust



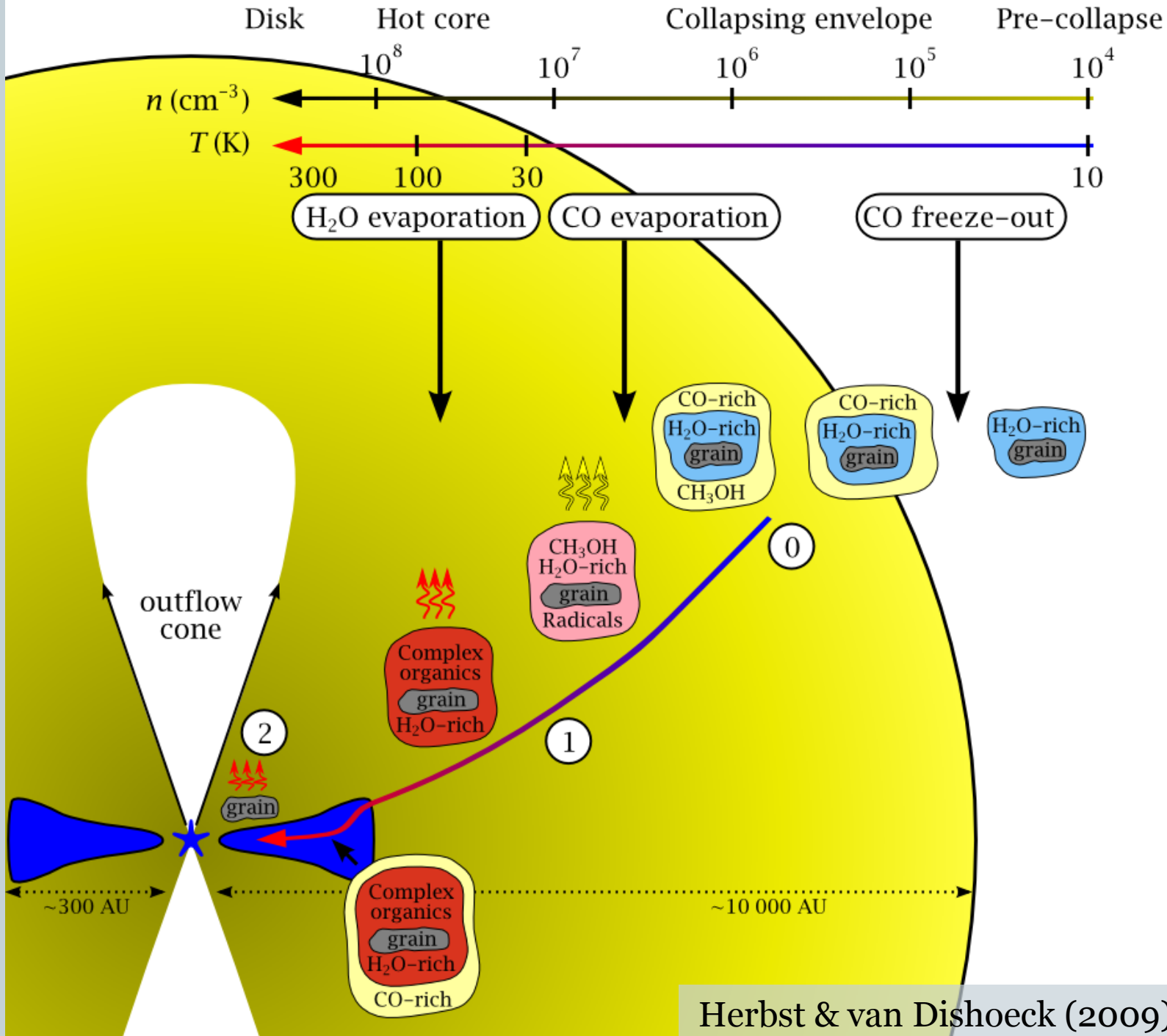
Low-mass star formation



Evolution of gas and dust

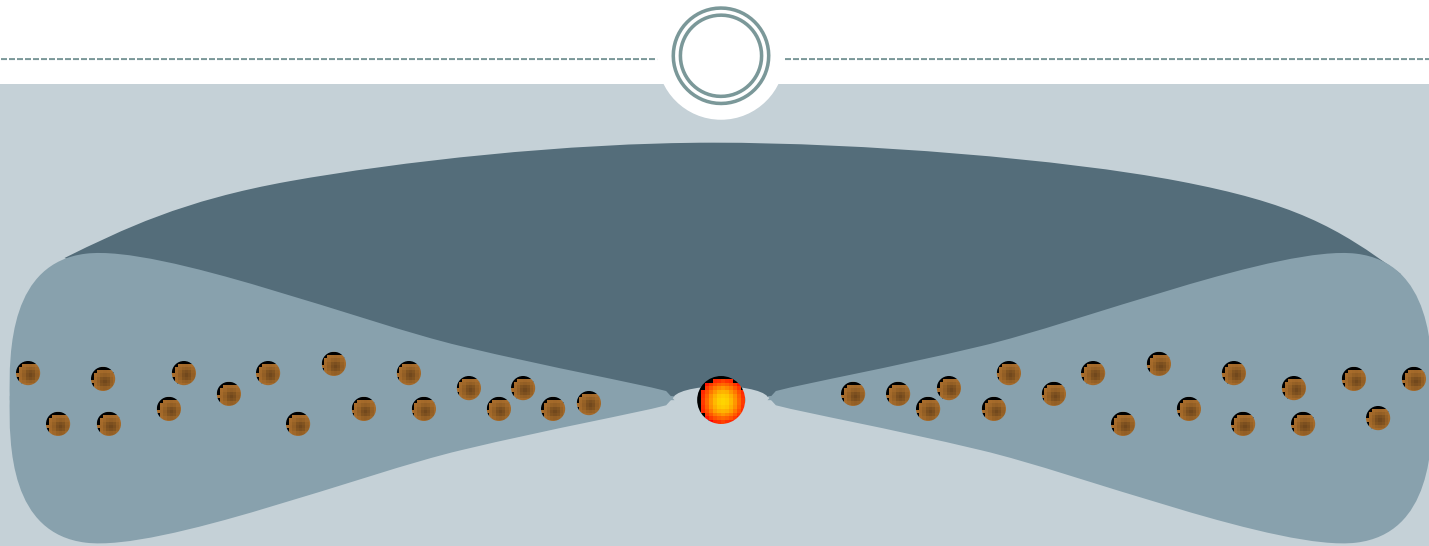
Low-mass star formation

Evolution of gas and dust



Herbst & van Dishoeck (2009)

T Tauri star and disk



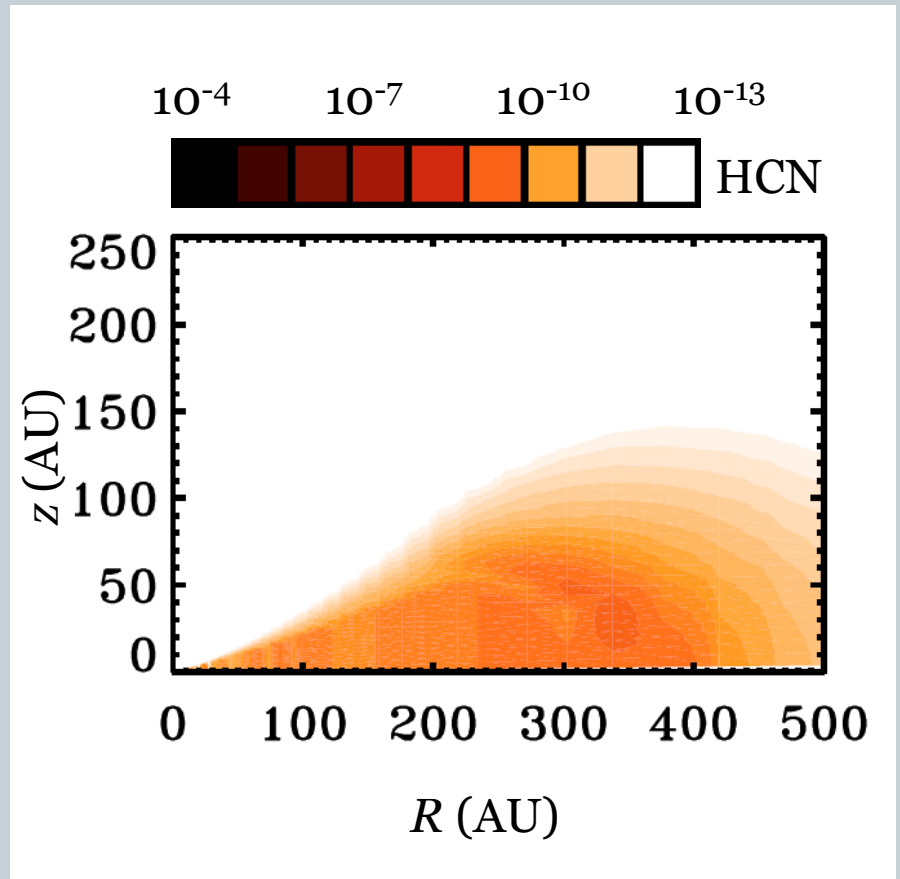
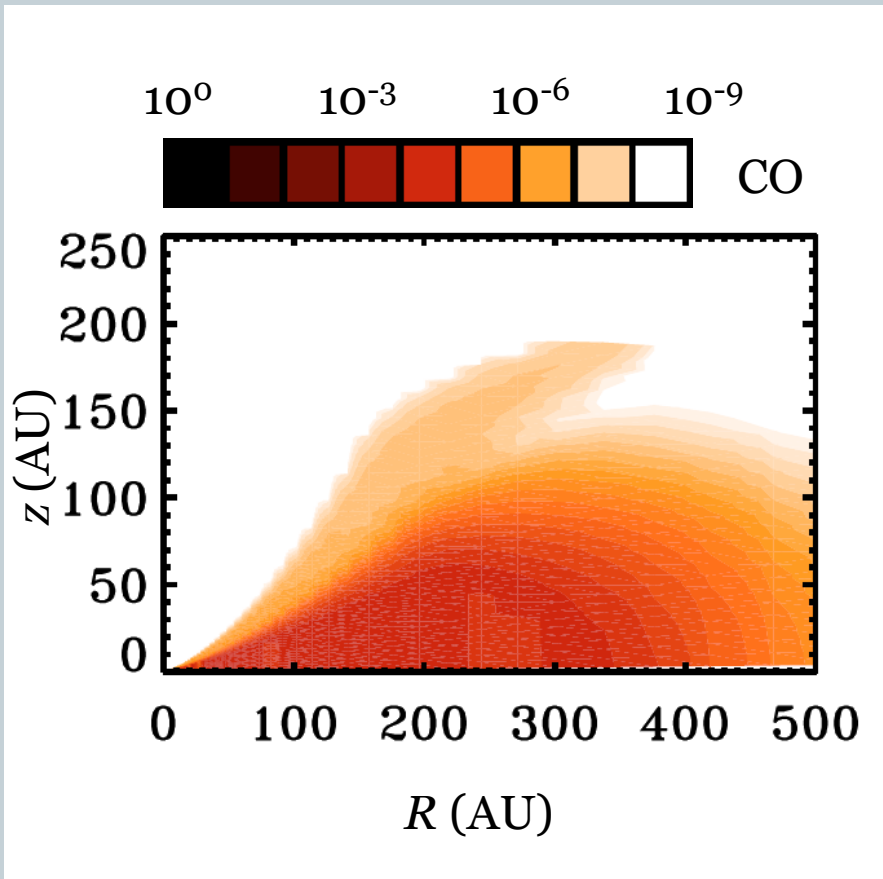
Star

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

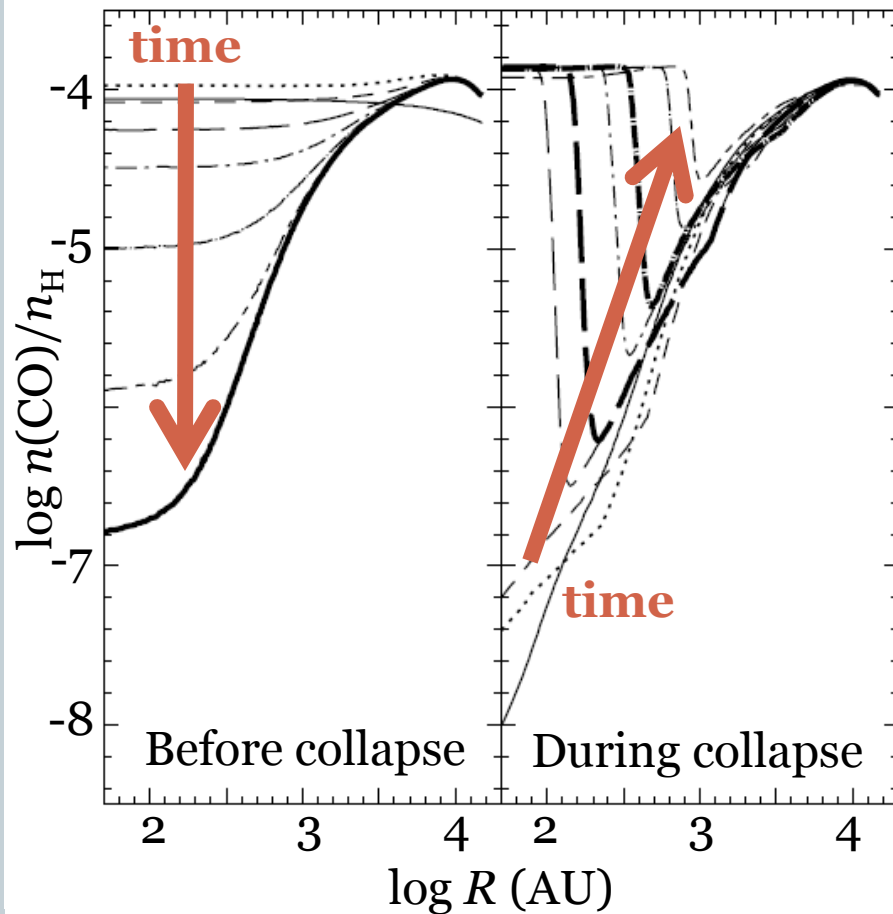
Disk

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

Chemistry in static disk models



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

Open questions

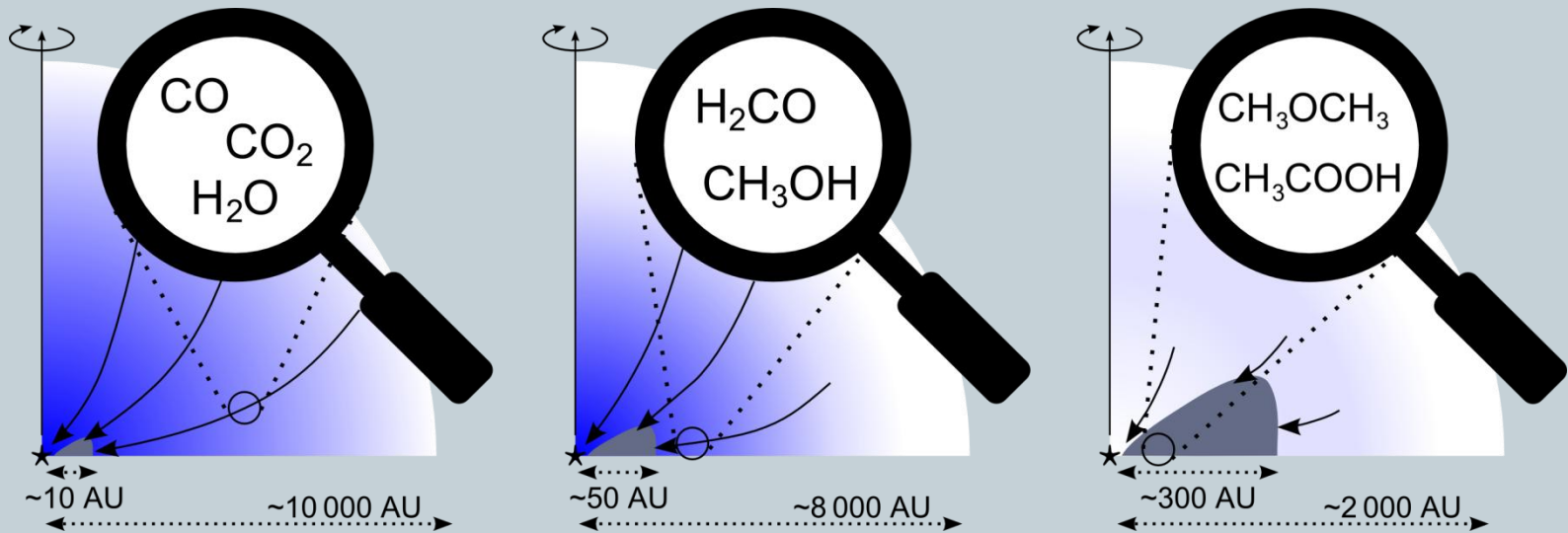


- When is the disk first formed?
- How do its size and mass evolve?
- How does material flow onto it from the envelope?
 - Onto hot inner parts or cold outer parts?
- How does the gas evolve?
 - Temperature, chemical composition, ...
- How does the dust evolve?
 - Size, amorphous or crystalline, ice mantle, ...
- What fraction of cometary ices is truly pristine?

Main features of this study



- One model from pre-stellar core to circumstellar disk
- Two-dimensional, axisymmetric
- Study chemical evolution
 - Composition of cometary and planetary building blocks
 - Chemistry affects physics: temperature, MRI, GI, ...
 - Diagnostic tool

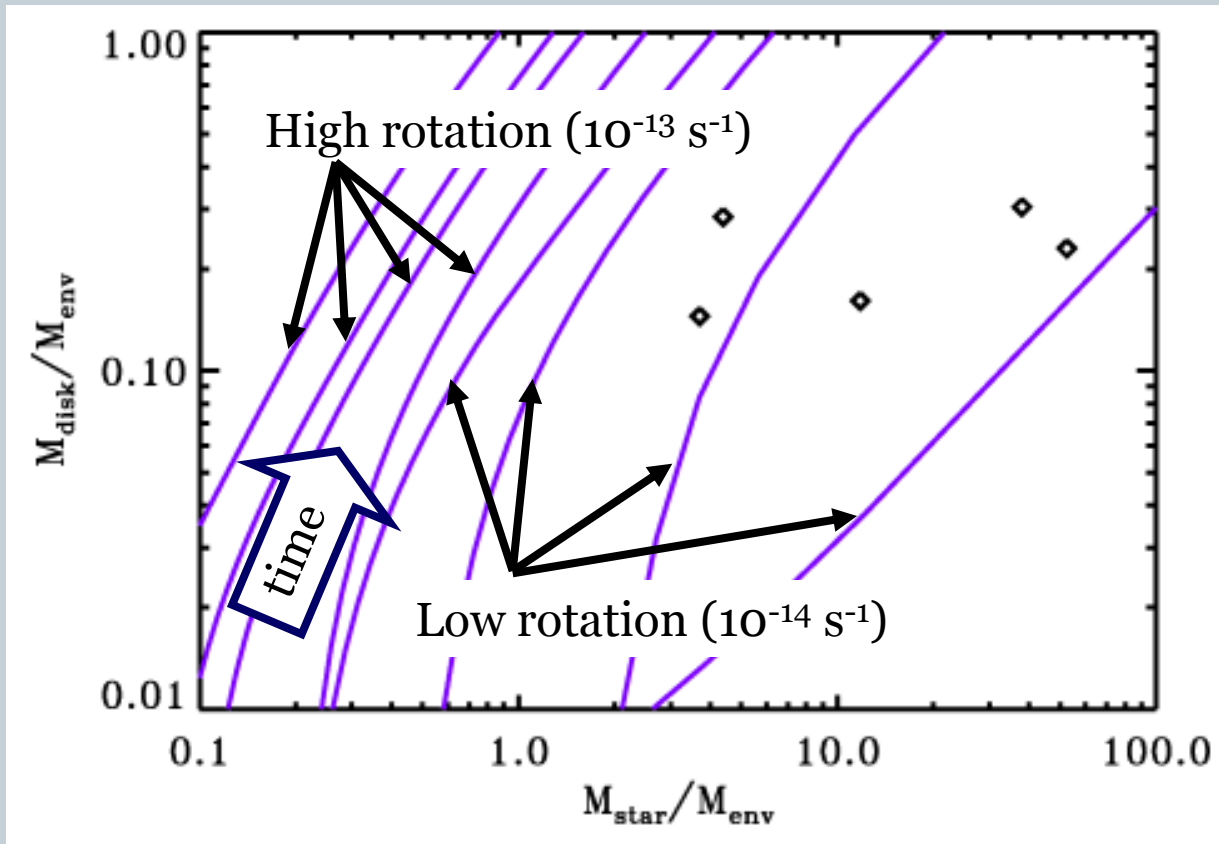


Analytical star formation model in 2D



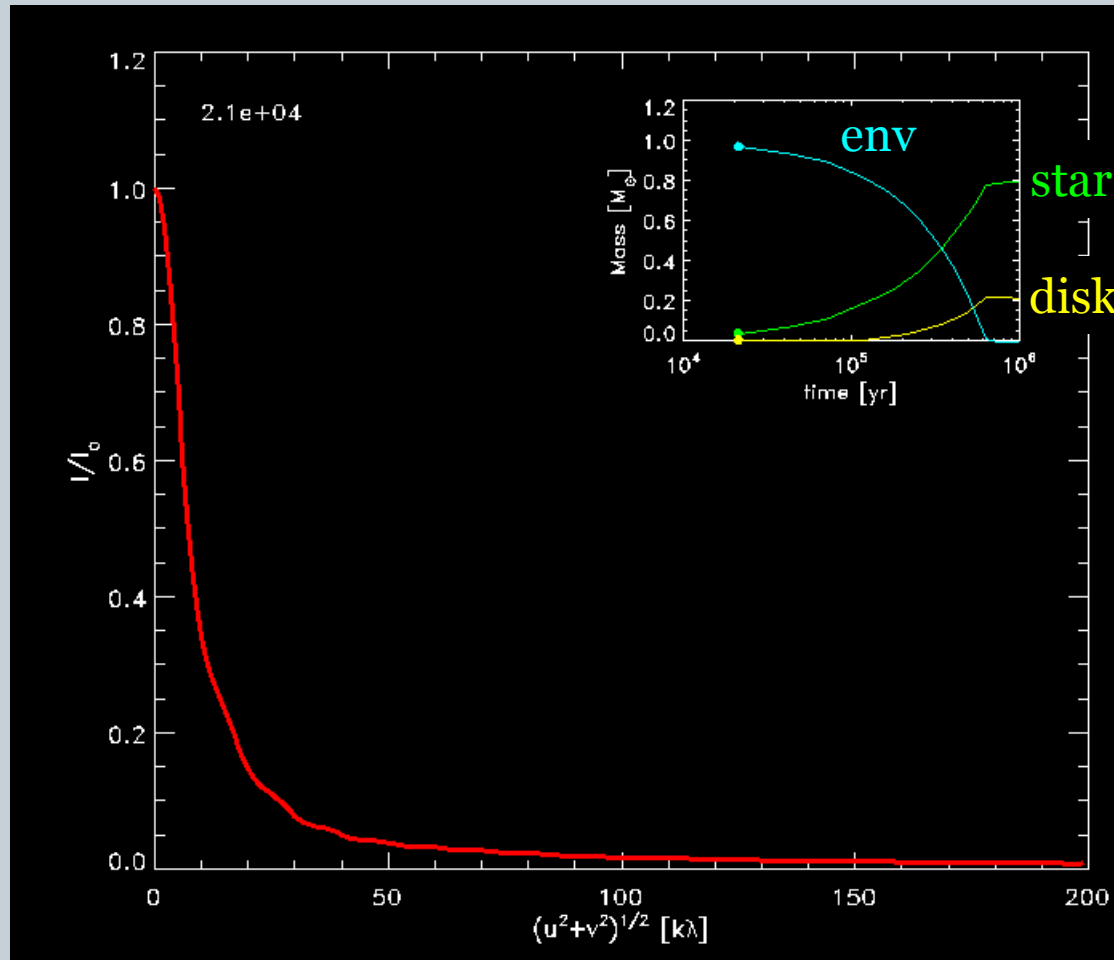
- Fast to run, high resolution,
easy to change initial conditions
Cloud mass (M_{\odot}), rotation rate (Ω_{\odot}), sound speed (c_s), ...
- Density & velocity: inside-out collapse
Shu (1977), Terebey, Shu & Cassen (1984)
- Dust temperature (important!) from
full radiative transfer
RADMC: Dullemond & 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

Model vs. observations: masses



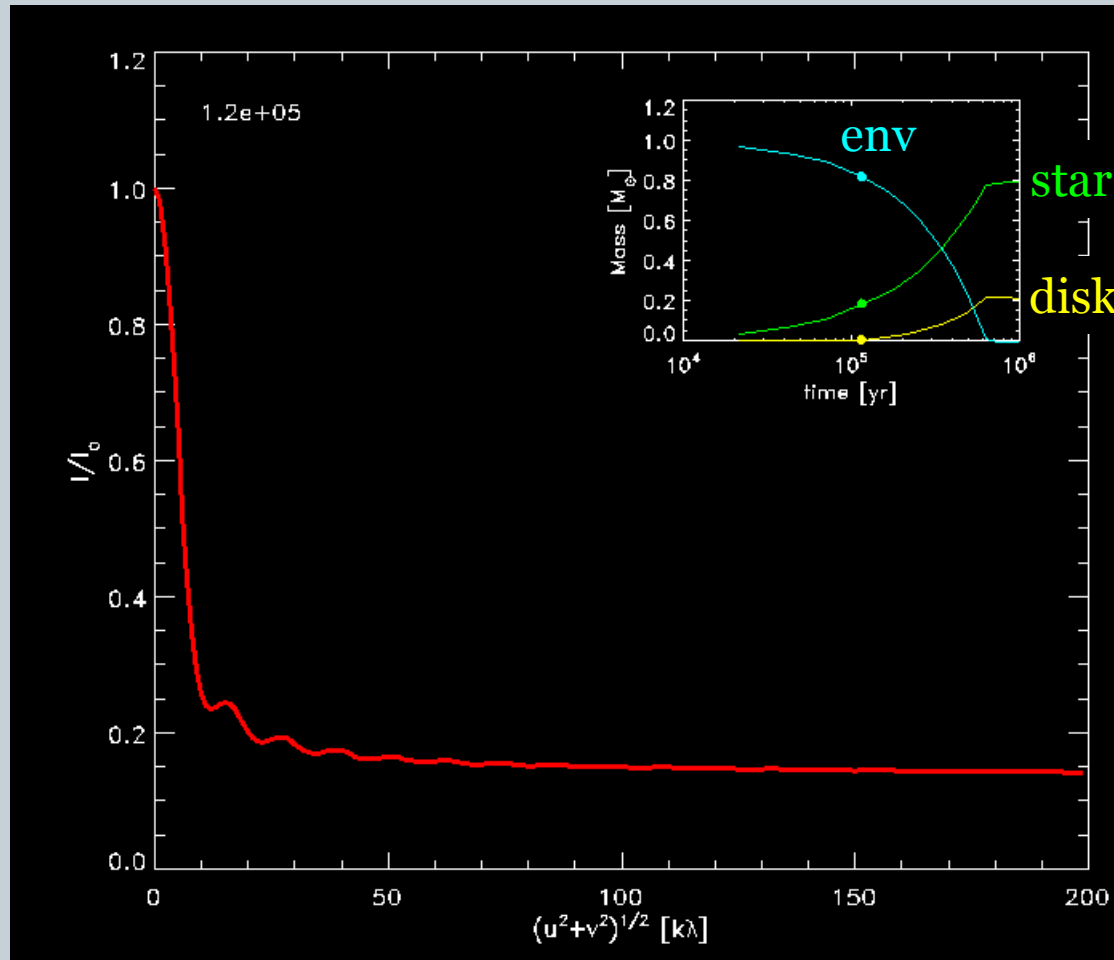
- Lines: model with different initial conditions
- Points: SMA observations
- Model over-predicts disk mass

Sub-mm model visibilities



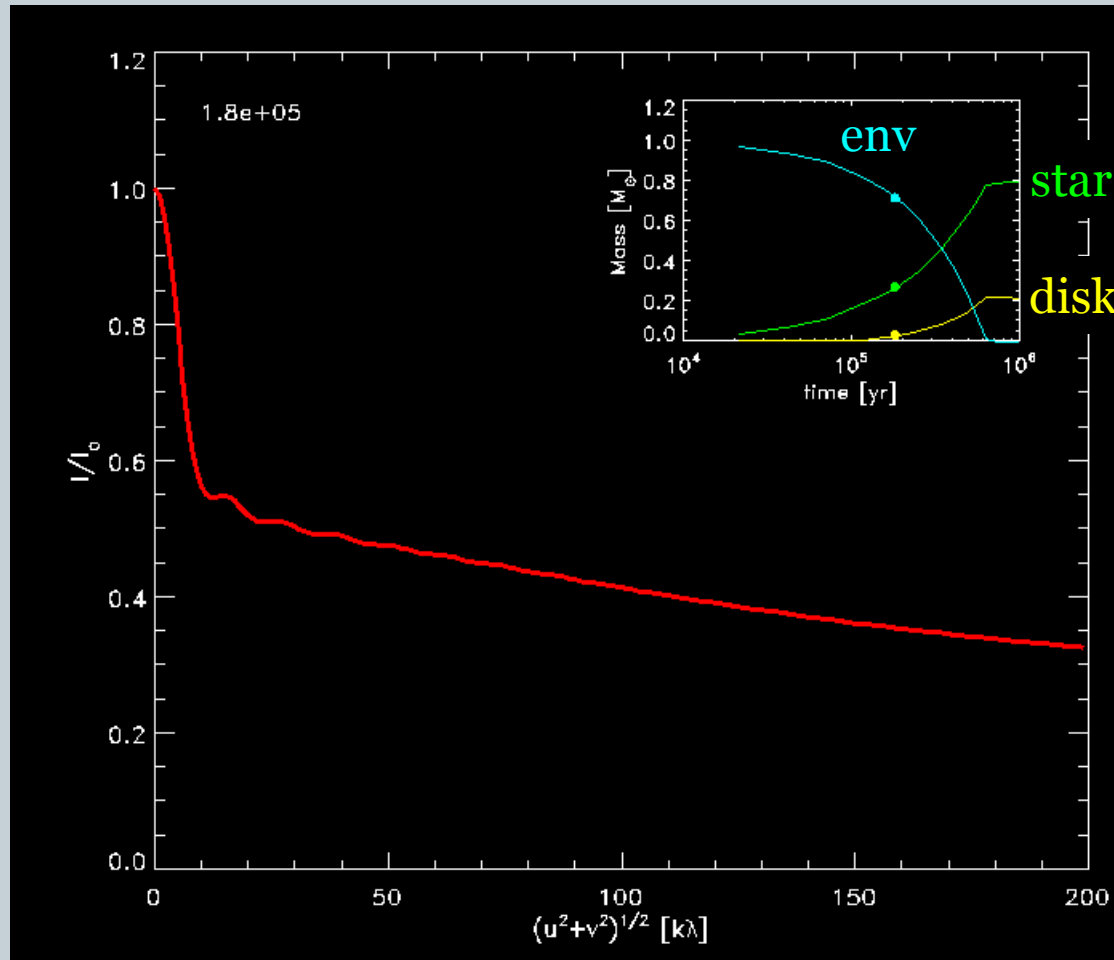
short baselines
=
large spatial
scales

Sub-mm model visibilities



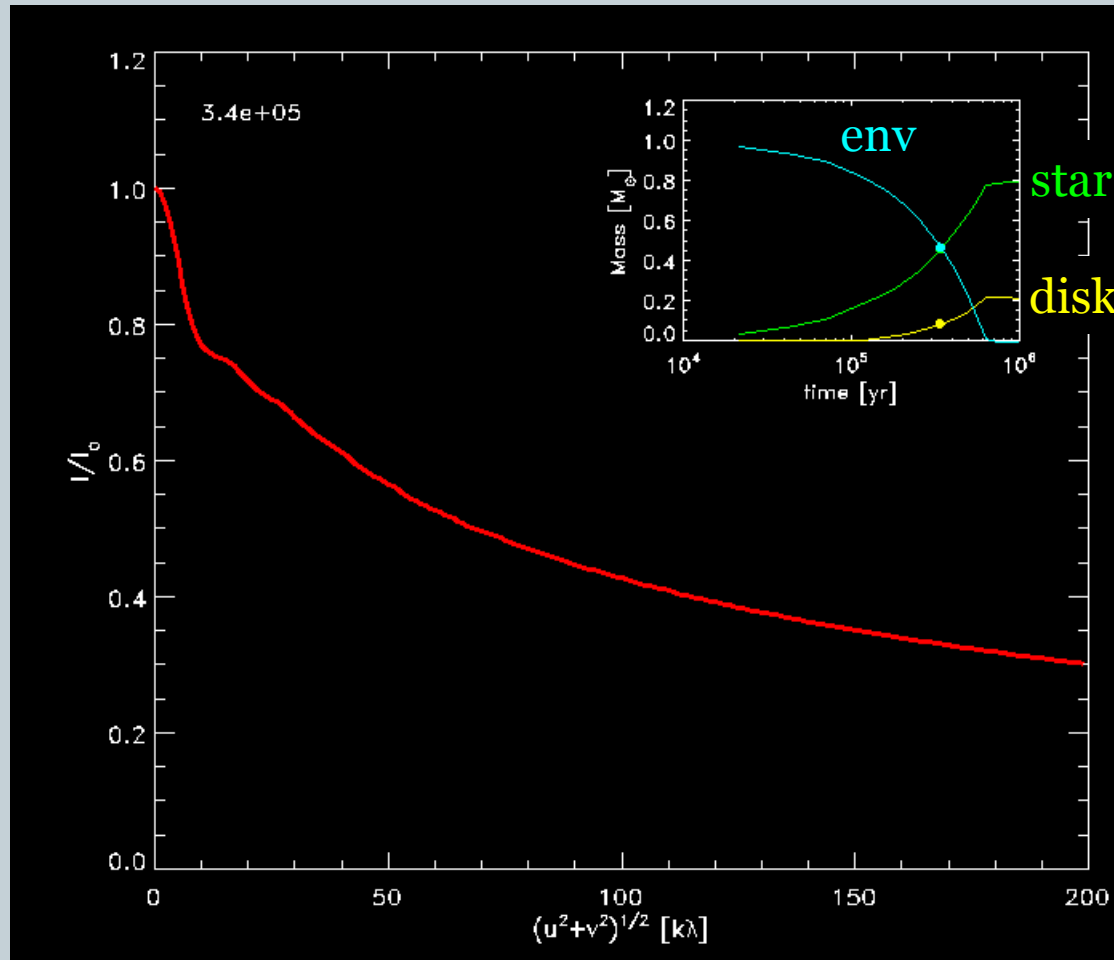
short baselines
=
large spatial
scales

Sub-mm model visibilities



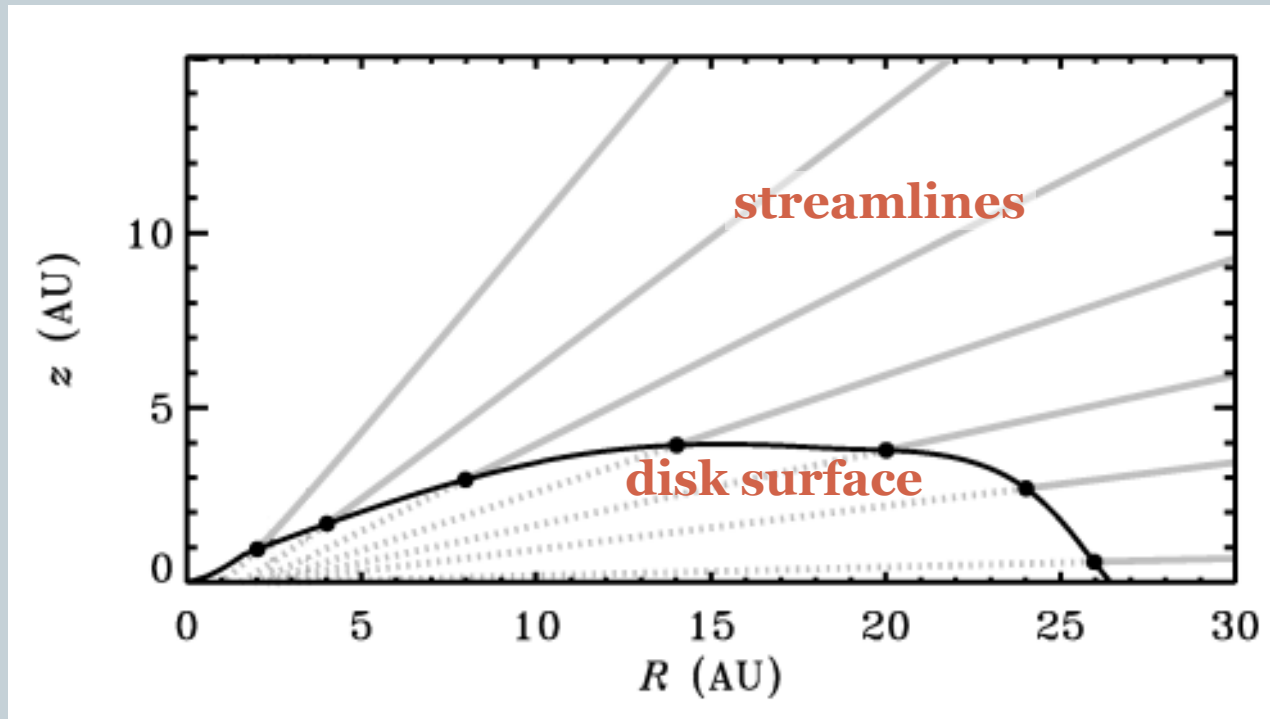
short baselines
=
large spatial
scales

Sub-mm model visibilities



short baselines
=
large spatial
scales

From one to two dimensions

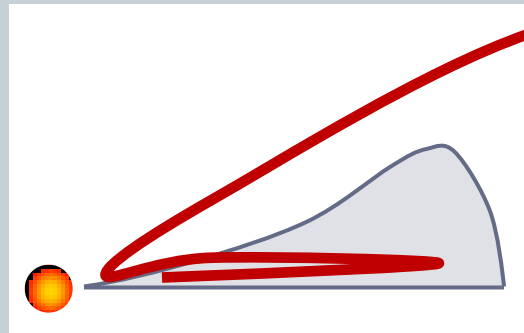
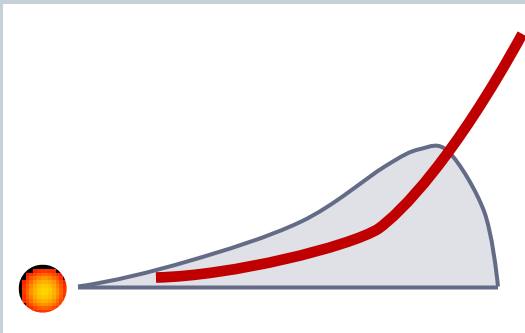


- Previous collapse models treated disk as completely flat
- Include vertical structure: accretion occurs further out
- Accretion shock is weak, except in very inner part

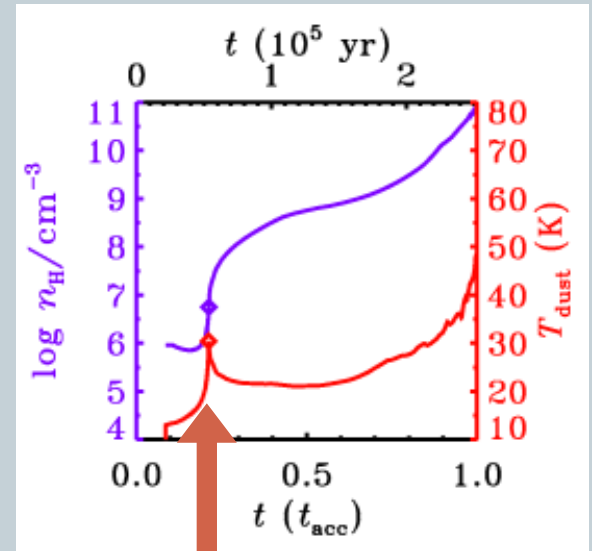
Infall trajectories



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



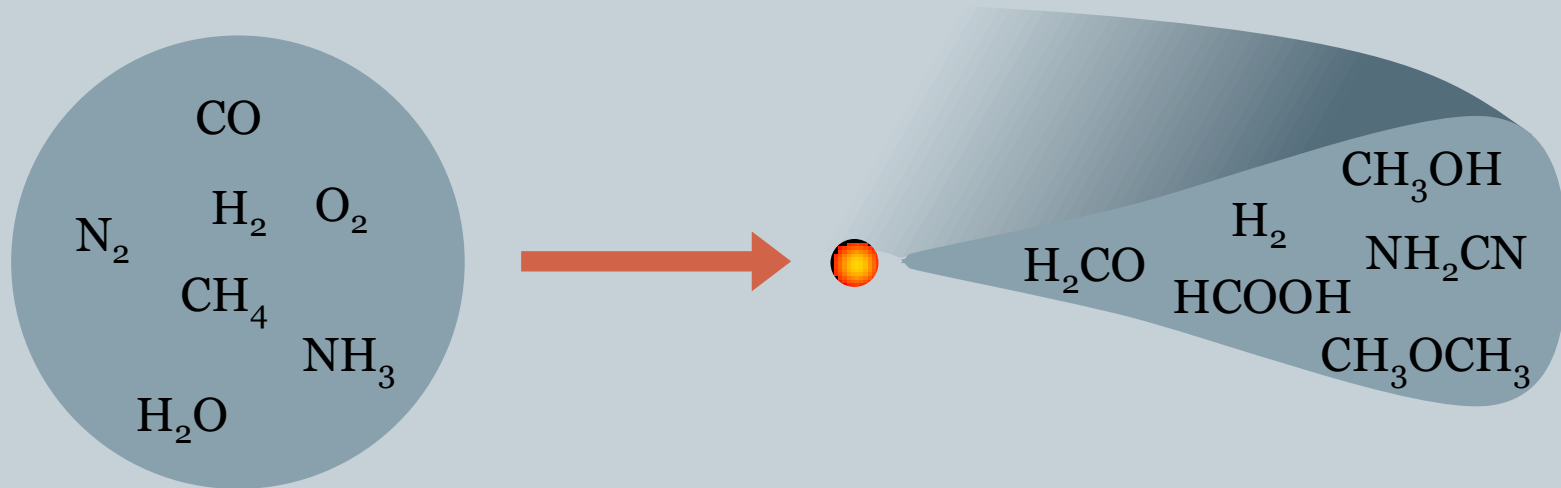
- Different trajectory shapes
- Jump in n , T upon entering disk



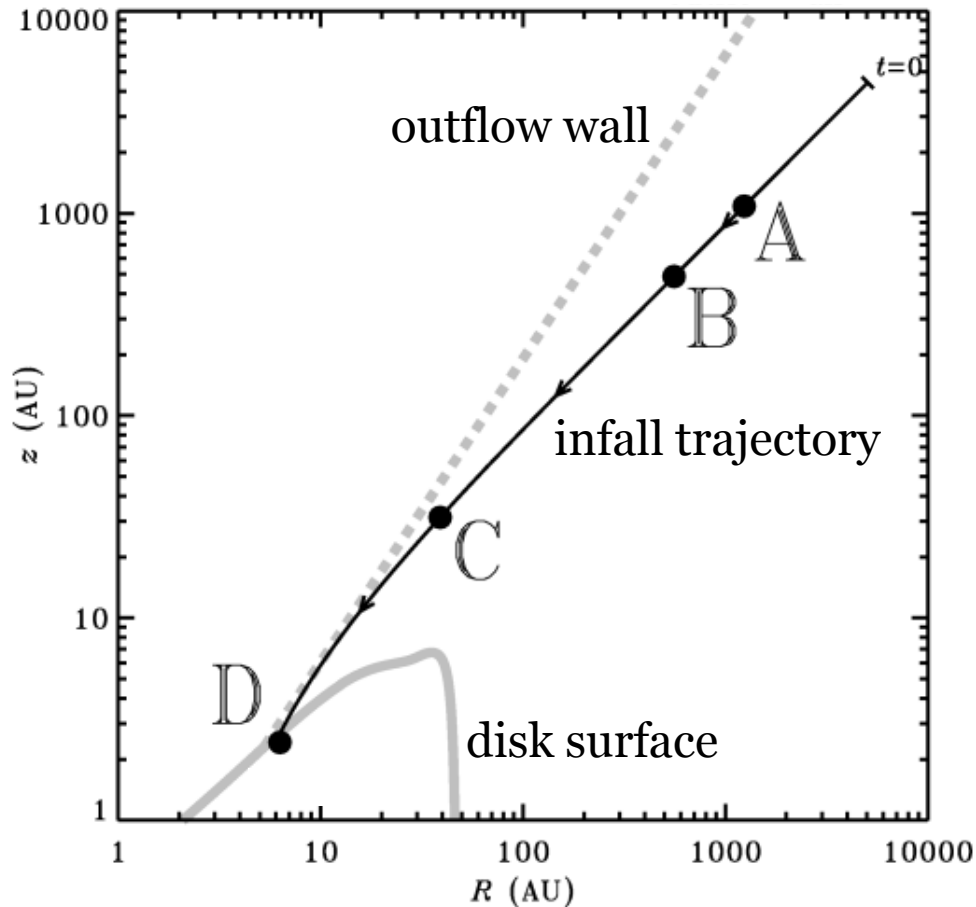
Full chemical model



- ~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



Chemical evolution along one trajectory



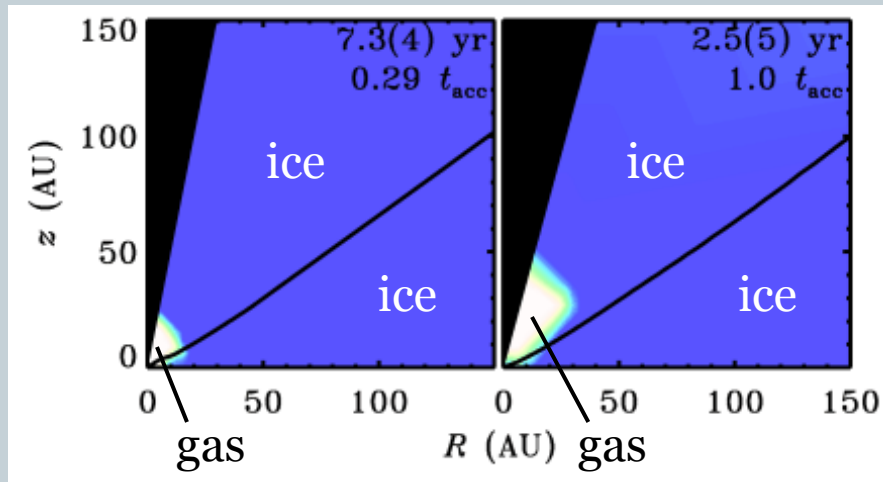
A: volatiles evaporate
(e.g. CO, N₂)

B: intermediates evaporate
(e.g. CH₄, NO)

C: other ices evaporate
(e.g. H₂O, NH₃, CH₃OH)
photodissociation of
many species

D: some species reformed

Gas and ice: H₂O

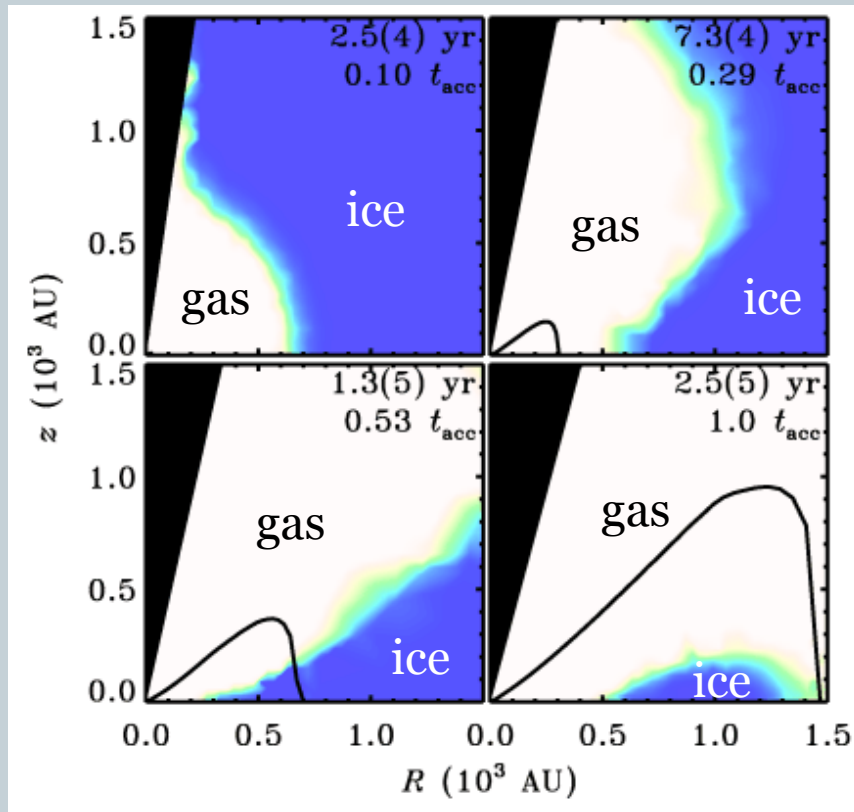


blue: all ice
white: all gas
black: outflow
black curve: disk surface

$$M_o = 1.0 M_{\text{sun}}$$
$$\Omega_o = 10^{-13} \text{ s}^{-1}$$
$$c_s = 0.26 \text{ km s}^{-1}$$

- H₂O remains solid except inner ~5 AU
- H₂O in comet-forming zone, depending on parameters:
 - *either* unprocessed
 - *or* evaporated and re-frozen

Gas and ice: CO

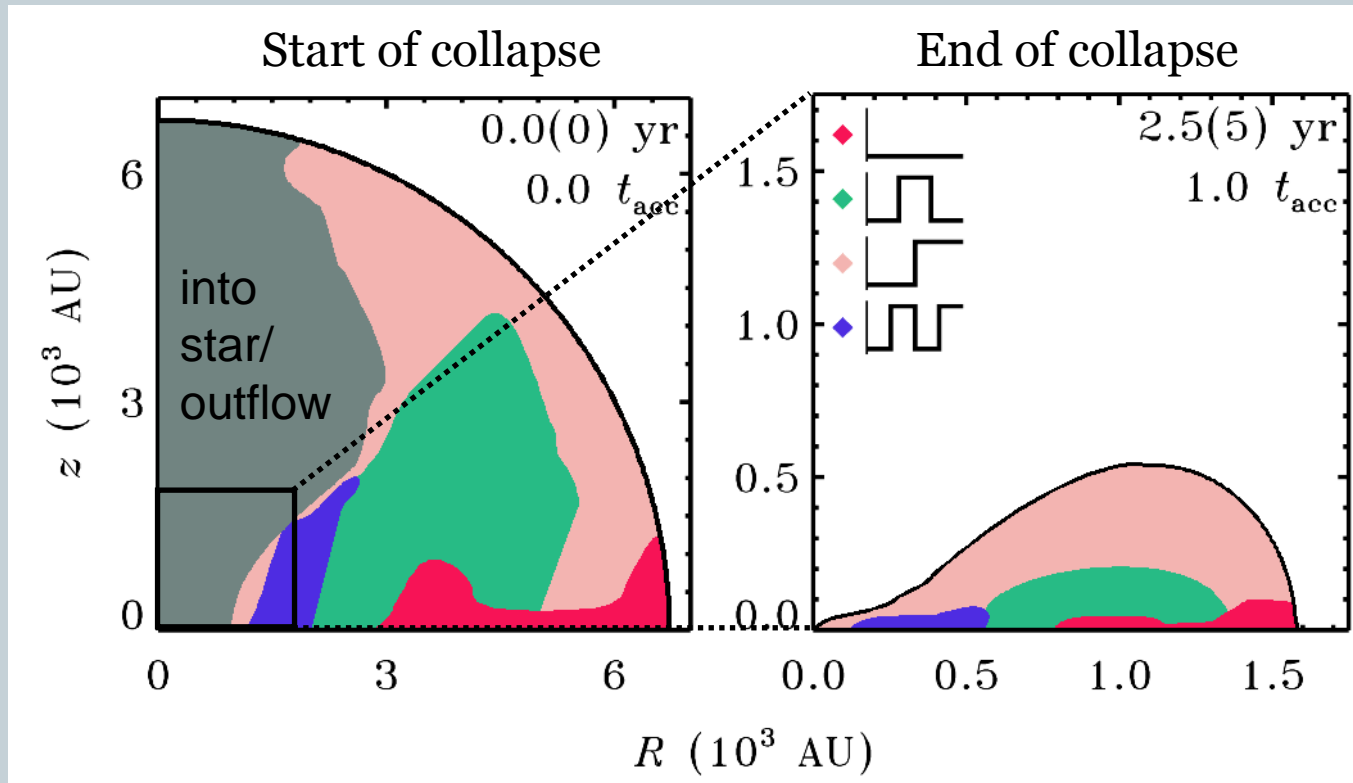


blue: all ice
white: all gas
black: outflow
black curve: disk surface

$$M_{\text{O}} = 1.0 M_{\text{sun}}$$
$$\Omega_{\text{O}} = 10^{-13} \text{ s}^{-1}$$
$$c_{\text{s}} = 0.26 \text{ km s}^{-1}$$

CO desorbs during infall, re-adsorbs in disk below 18 K

Chemical zones: CO gas/ice



$$M_o = 1.0 M_{\text{sun}}$$
$$\Omega_o = 10^{-13} \text{ s}^{-1}$$
$$c_s = 0.26 \text{ km s}^{-1}$$

Red: CO remains adsorbed (pristine!)

Green: CO desorbs and re-adsorbs

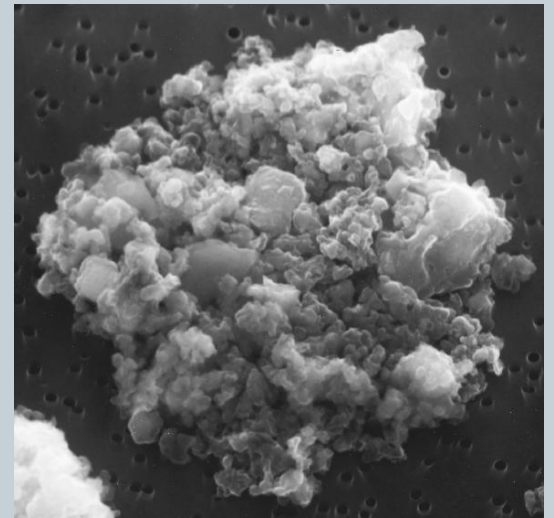
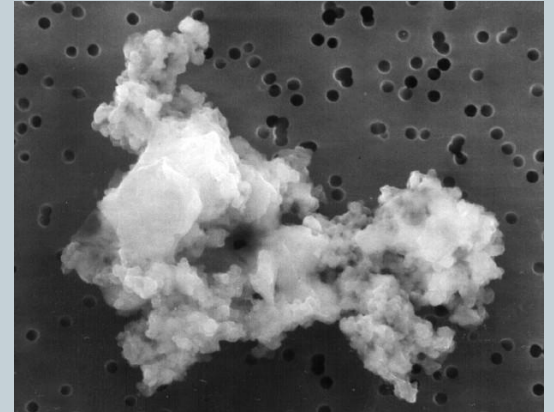
Pink: CO desorbs and remains desorbed

Blue: multiple desorption/adsorption

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 , ...



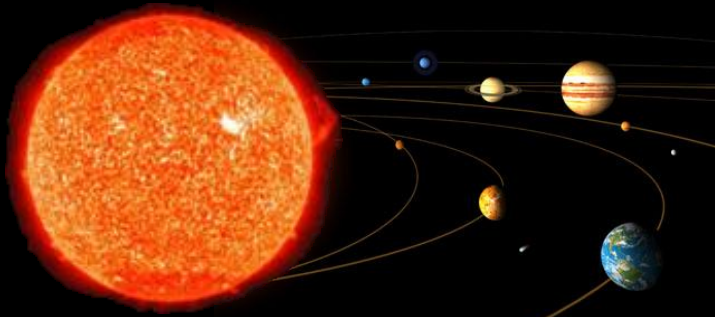
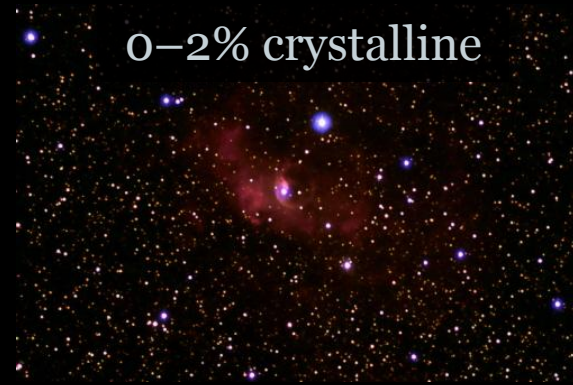
From crystalline to amorphous and back



up to 50% crystalline



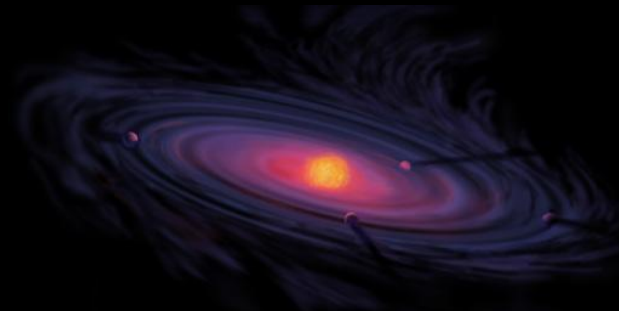
0–2% crystalline



up to 50% crystalline



1–30% crystalline



Origin of crystalline silicates in disks



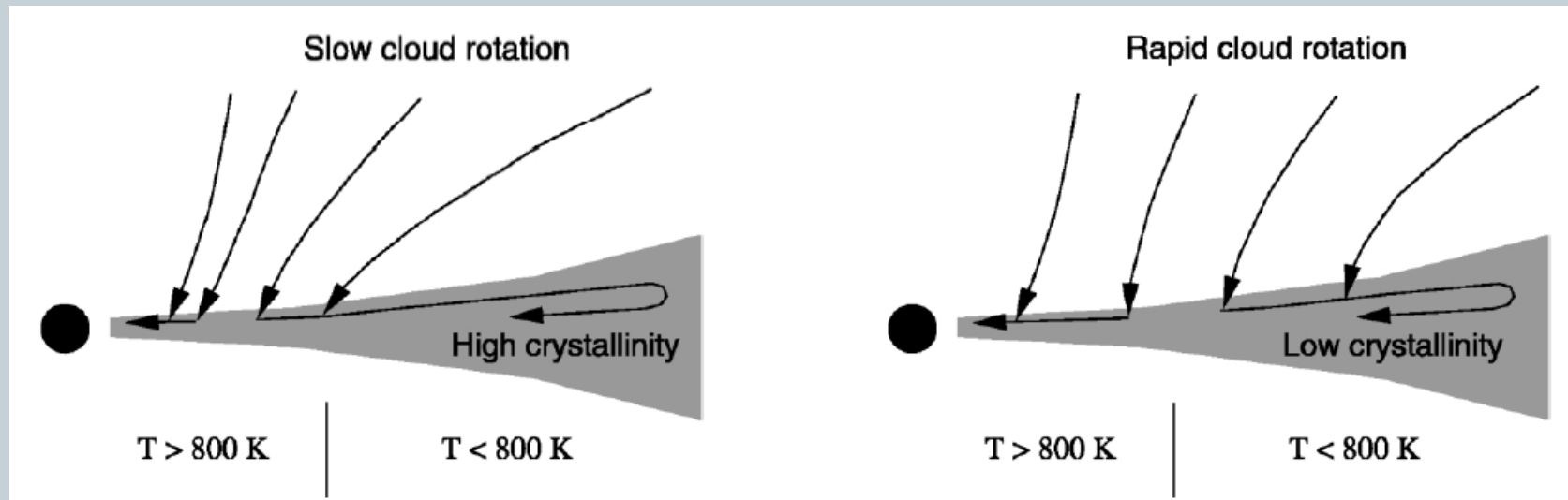
- Crystallization by thermal annealing requires 800 K
- Crystalline silicates observed down to 150 K
- Bouwman et al. (2008): enstatite/forsterite ratio depends on radius

- Transport from hot inner parts to cold outer parts?
 - Nuth 1999, Bockelée-Morvan et al. 2002, Keller & Gail 2004
- Local heating by shocks?
 - Harker & Desch 2002, Desch et al. 2005

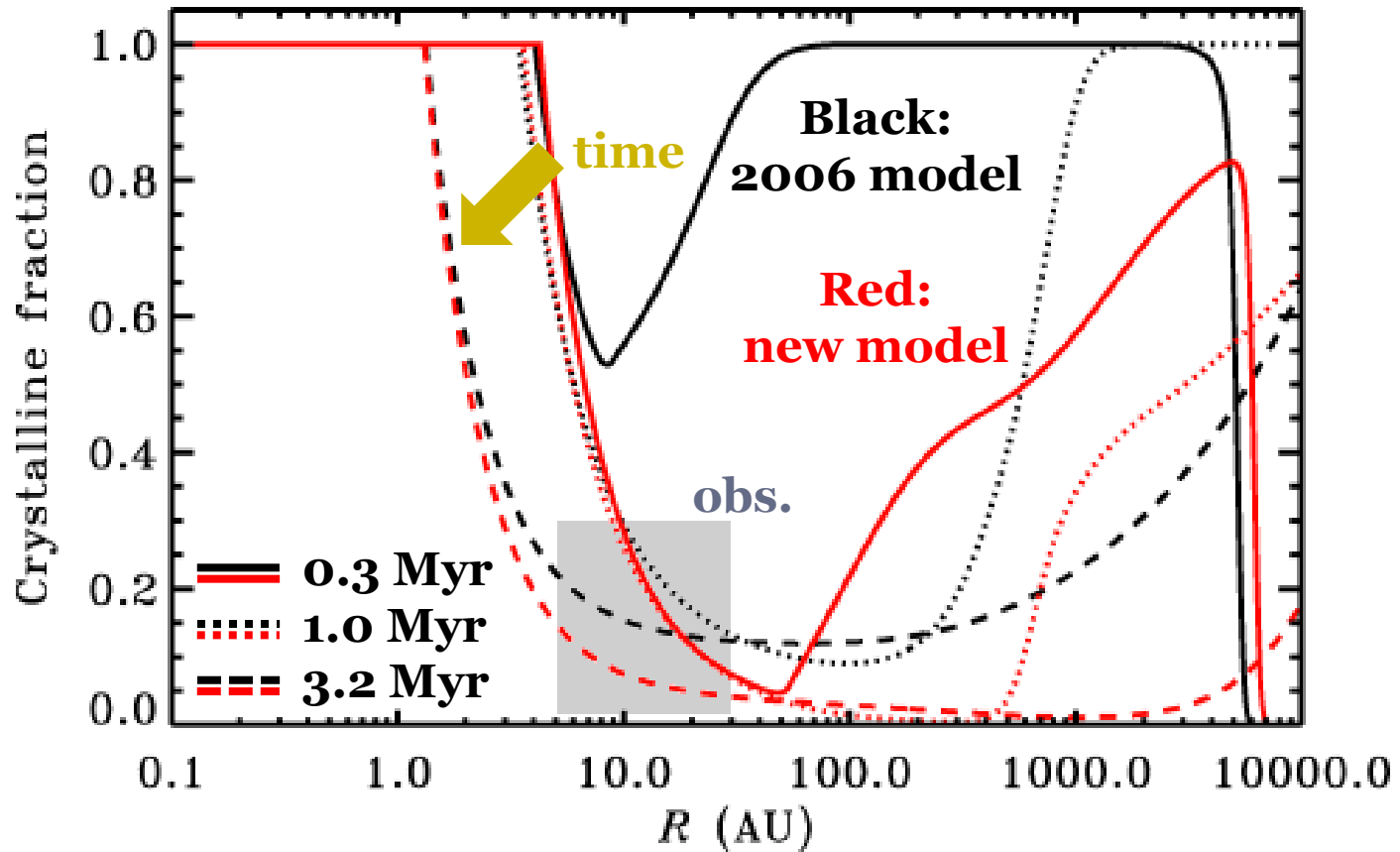
Disk evolution model



- 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



Crystalline fractions



Model results in good agreement with observed range!

Implications for comets



Observations

- Silicate dust
 - Partially crystalline
 - Partially amorphous
- Chemical composition
 - Generally similar to ISM
 - Individual differences

Model

- Silicate dust
 - Partially crystalline
 - Partially amorphous
- Chemical composition
 - Outer disk unprocessed
 - 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 , ...
- **Mixing**
 - Chemical zones in disk more diffuse

Conclusions



- First model to follow chemistry from pre-stellar cores to circumstellar disks in 2D
- Masses and densities compares well with hydro simulations and SMA observations
- Great tool for chemical evolution
- Disk is divided into zones with different chemical histories
 - Outer part pristine, inner part processed
- Thermal annealing followed by radial transport is responsible for at least part of observed silicates

Future work



- **Compute line profiles**
 - Compare with observations by SMA, JCMT, IRAM 30m, ...
 - Analyse water data from Herschel (WISH key program)
 - Make predictions for ALMA
- **Add grain-surface chemistry**
 - Formation of complex organics
- **Add isotope-selective CO photodissociation**
 - New model: Visser, van Dishoeck & Black (2009)
- **Quantify effects of mixing on chemistry**
 - Better match with cometary abundances?