The chemical history of molecules in circumstellar disks

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May 29, 2009

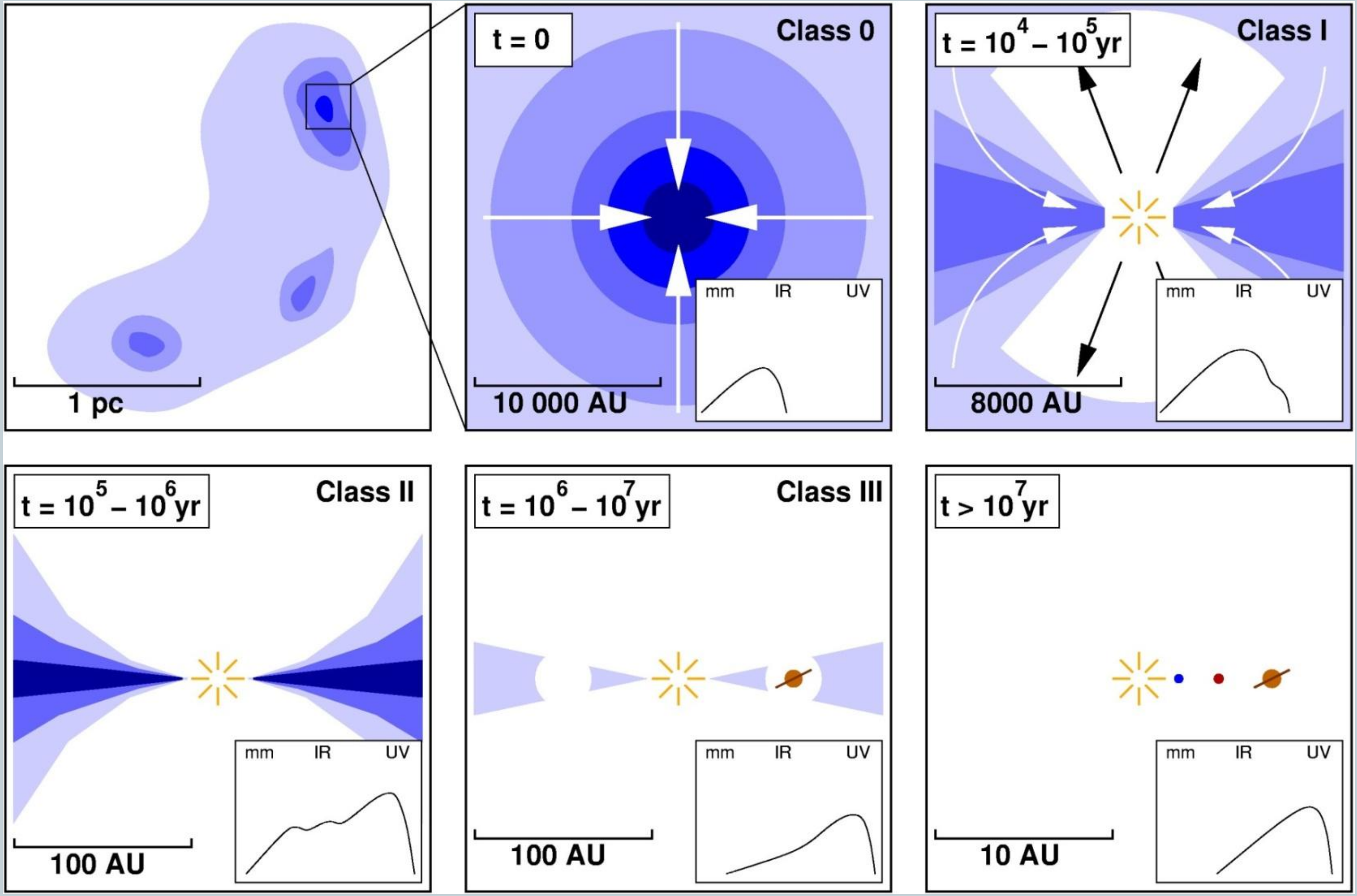
Astrochemistry and star formation in Leiden

- Observations
  - Spitzer, VLT, JCMT, IRAM, Herschel, ALMA, …
  - All stages of (low-mass) star formation
- Laboratory astrophysics
  - Simulate conditions in space, with main focus on ices
  - Desorption kinetics, surface reactions, photoprocessing
  - Complementary Monte Carlo simulations
- Theoretical models
  - Simulate star formation (hydrodynamically and analytically)
  - Radiative transfer
  - Chemical networks

Motivation for my project

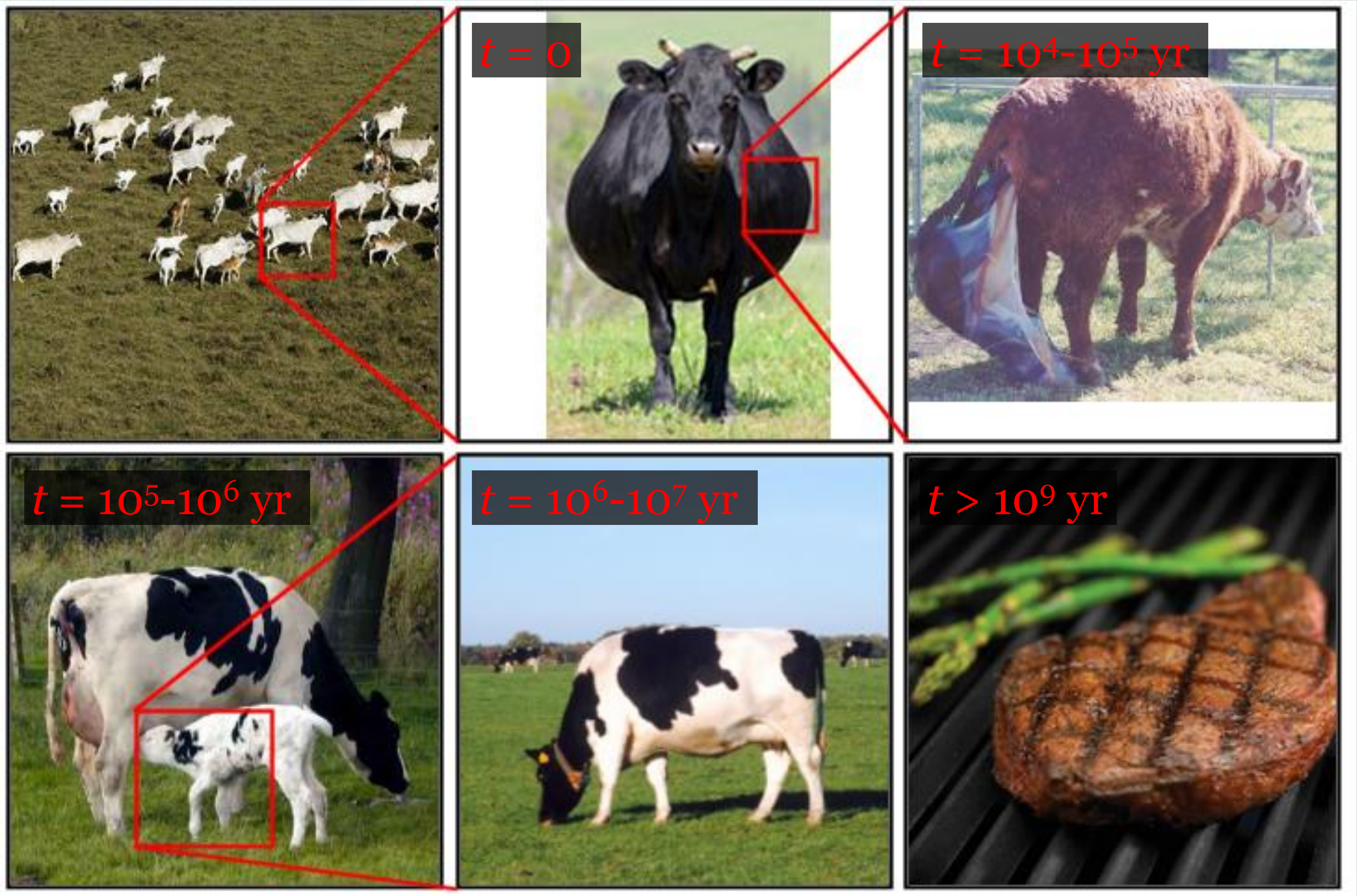
- Why circumstellar disks?
  - Origin of the solar system
  - Formation of different types of exoplanets
  - Feedback to interstellar medium
- Why chemical history?
  - Composition of planetary building blocks
  - Origin of life
  - Spectroscopic observations
  - Trace physical conditions
  - Effect on physics

Low-mass star formation

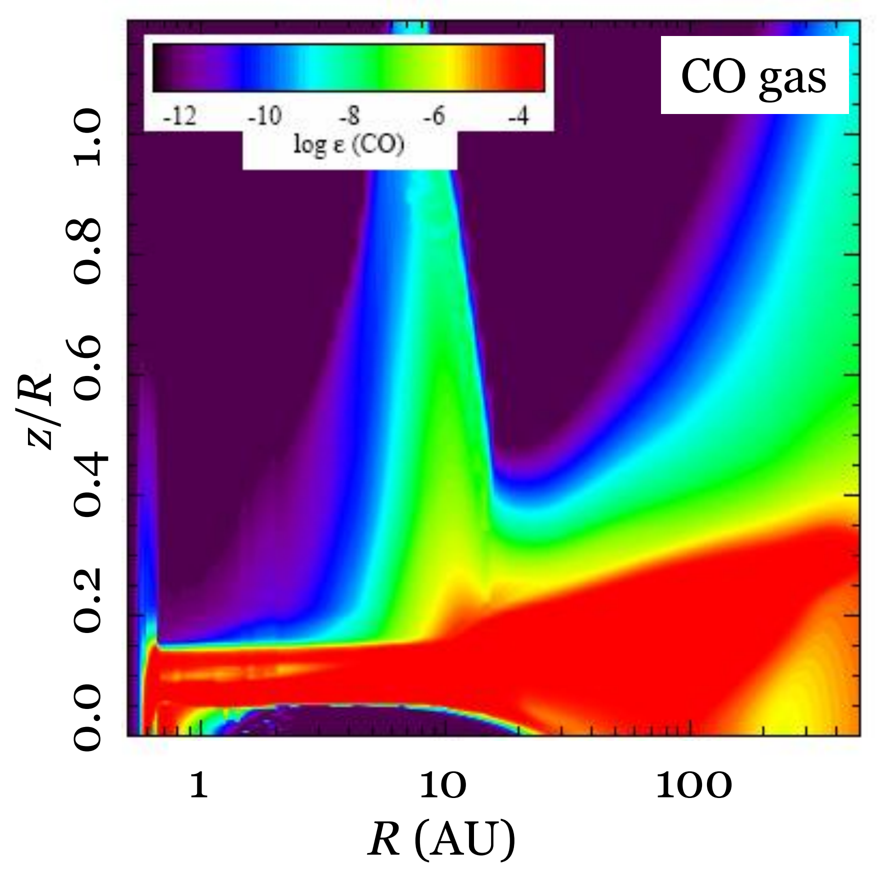


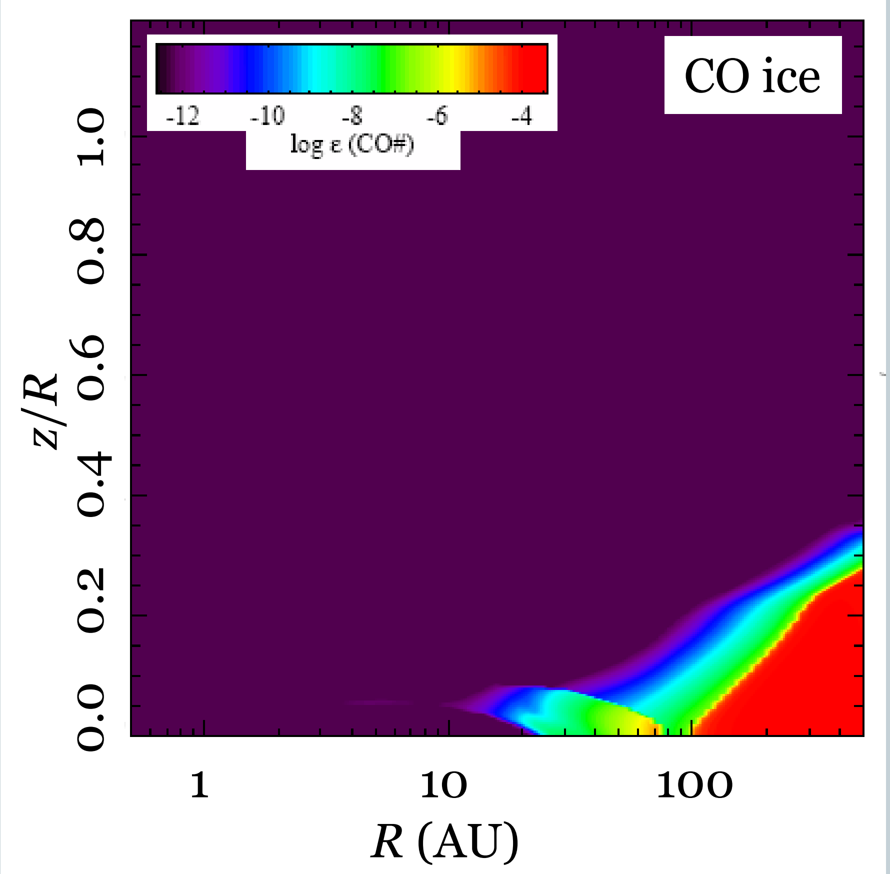
Jonkheid et al. 2006

Low-mass ~~star~~ cow formation



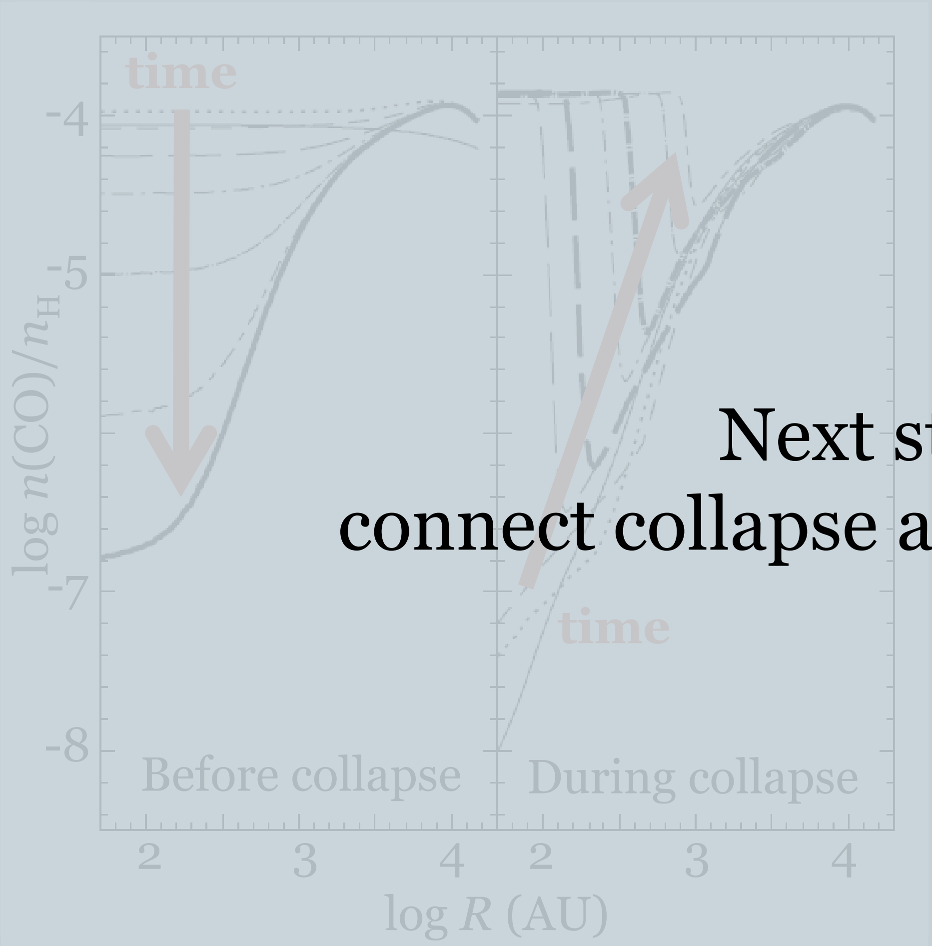
Chemistry in static disk models





Woitke, Kamp & Thi 2009

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

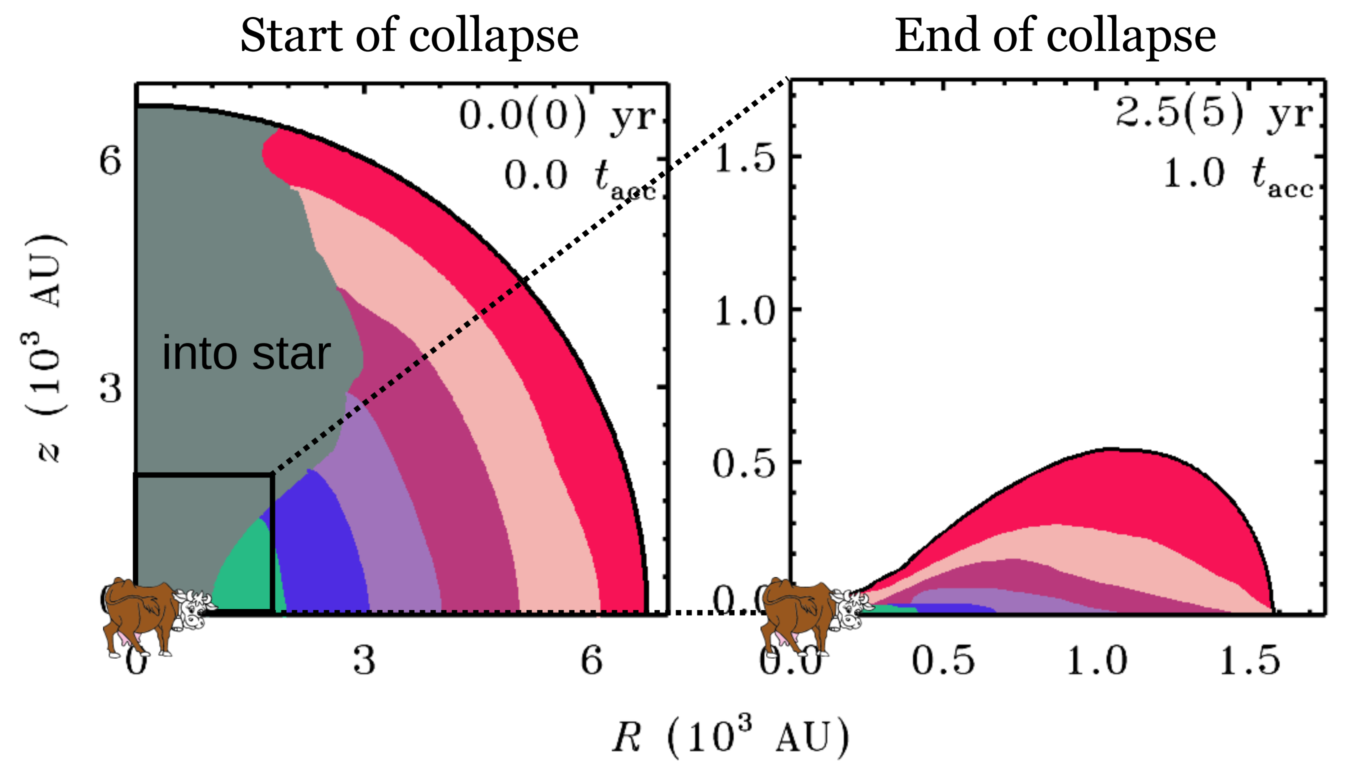
Lee, Bergin & Evans 2004

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 hydro models
  Yorke & Bodenheimer 1999, Brinch et al. 2008a,b
- Density profiles compare well with observations
  Jørgensen et al. subm.

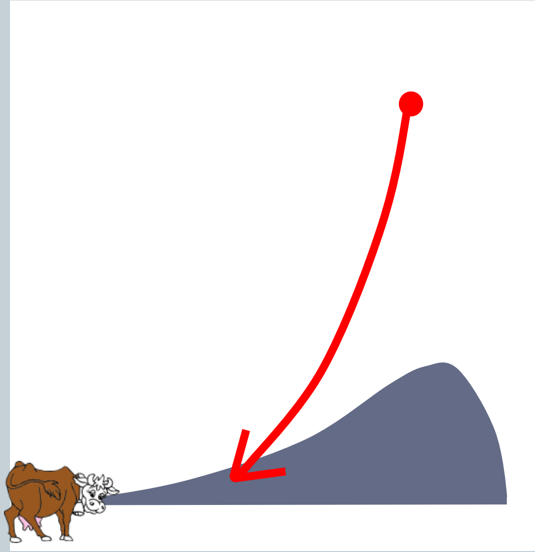
Where does material go to?

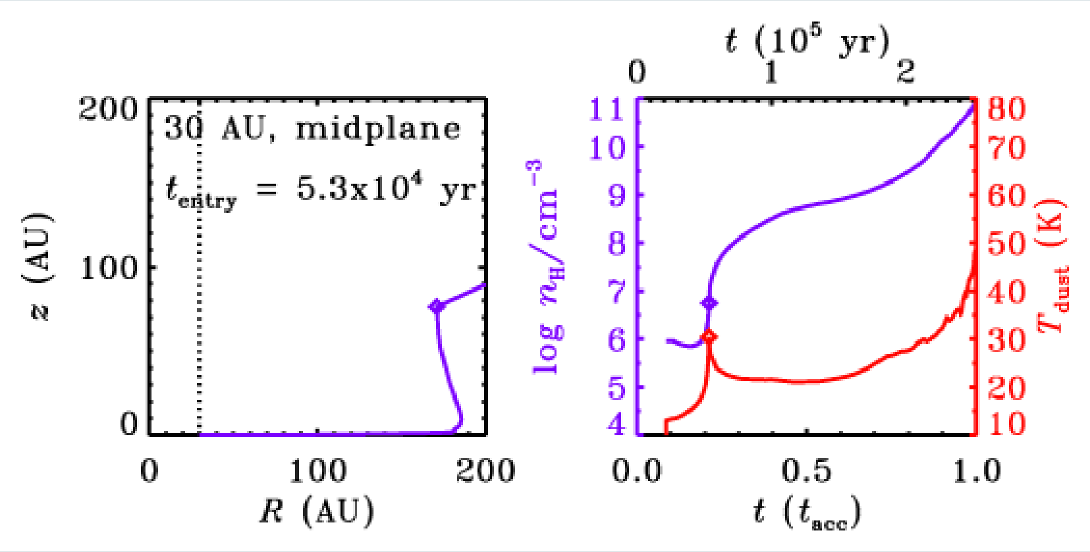
Inside-out collapse gives a layered disk



Infalling trajectories

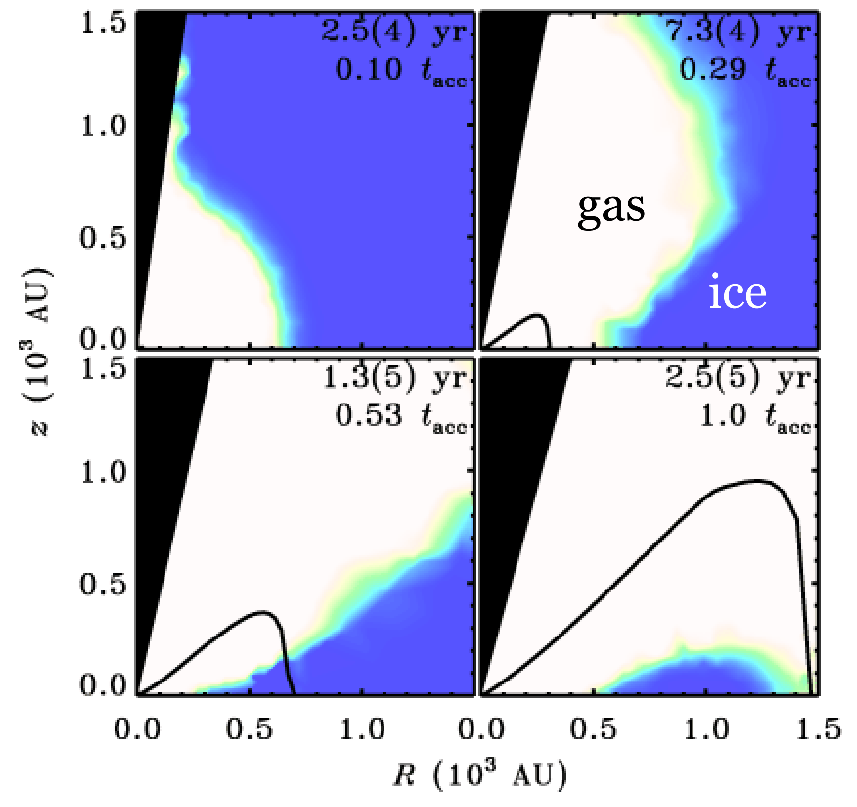
- Need to solve chemistry dynamically: compute n, T along many trajectories



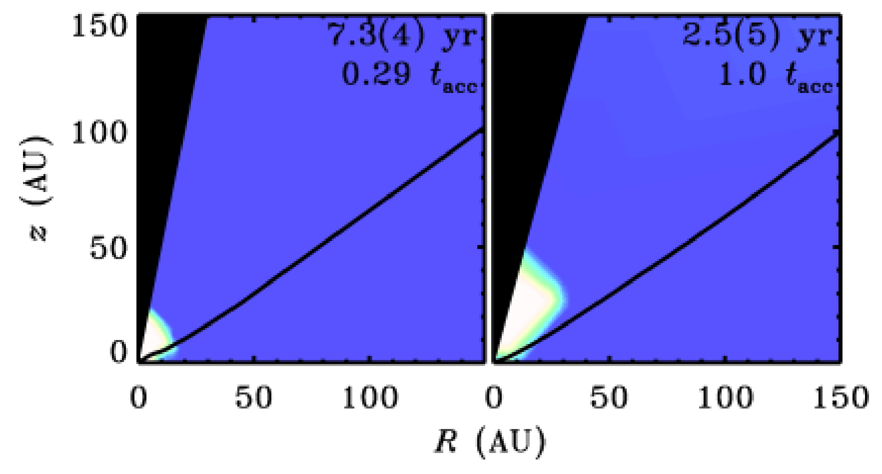


- Jump in n, T upon entering disk
- n increases by factor of ~10^5 overall, T goes from 10 to several 10s of K

Gas and ice



CO

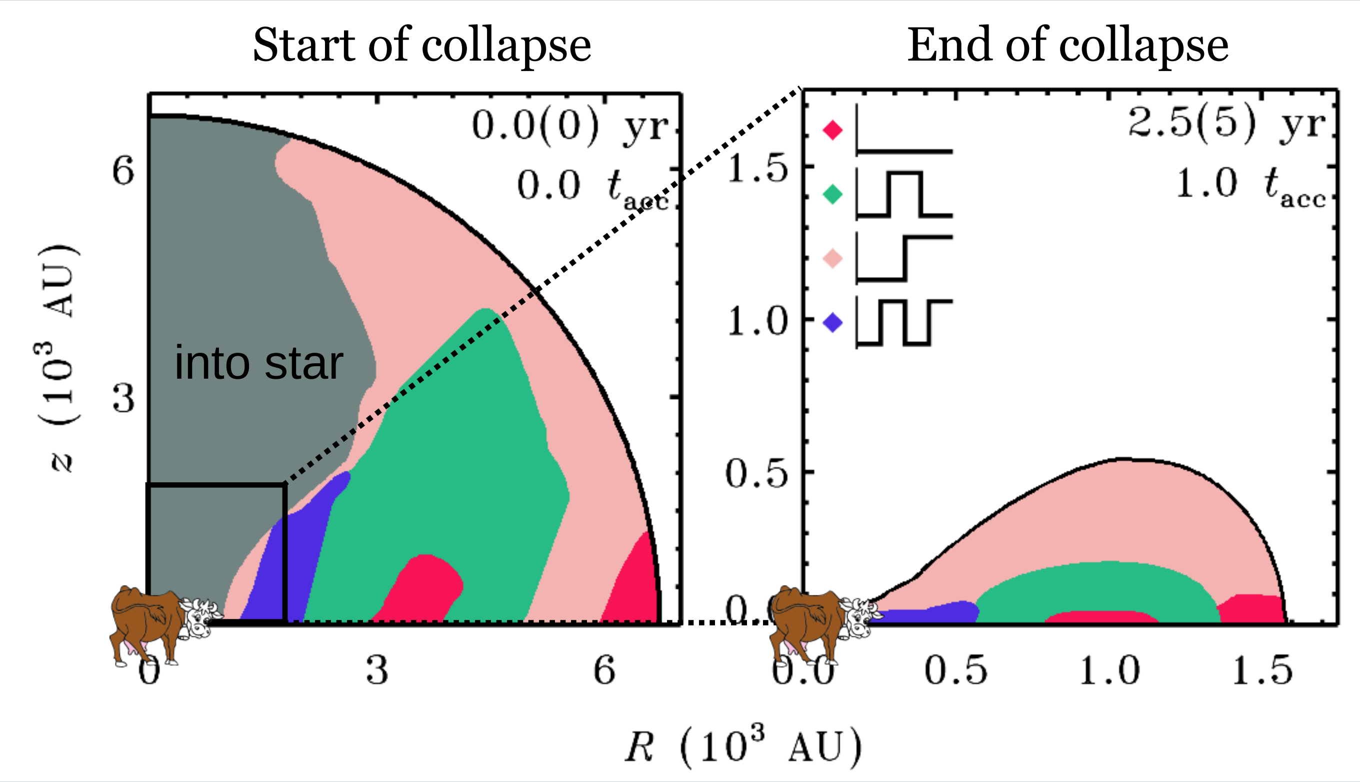


H_2O

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

Chemical zones: CO gas/ice



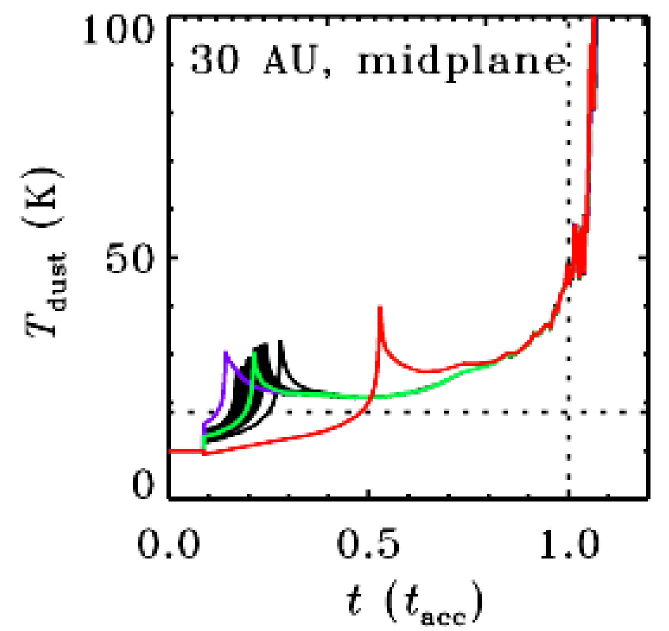
Red: CO remains adsorbed (pristine!)

Green: CO desorbs and re-adsorbs

Pink: CO desorbs and remains desorbed

Blue: multiple desorption/adsorption

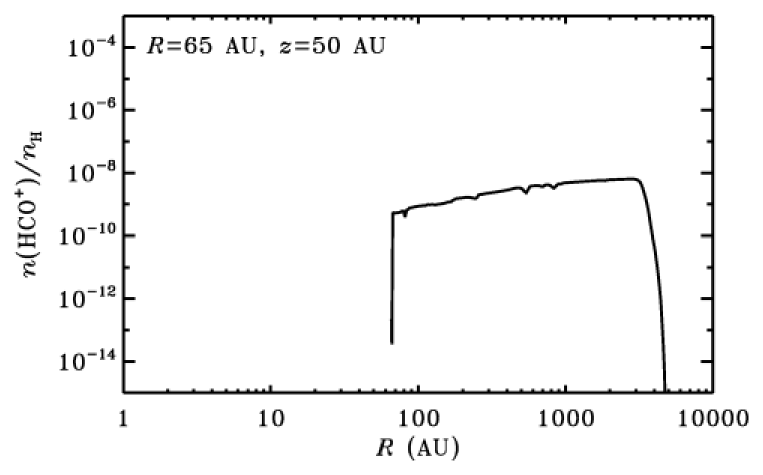
Complex organic molecules

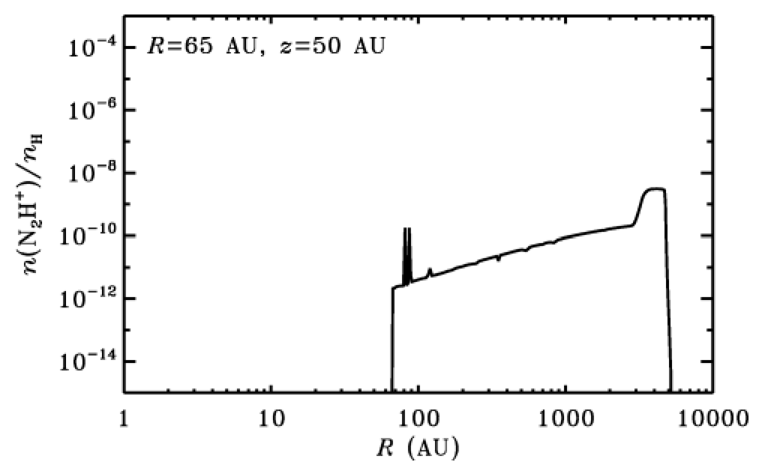


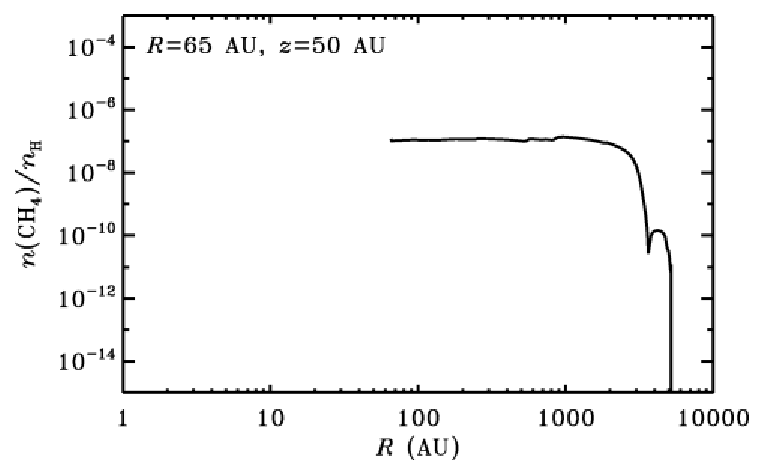
- First generation
  - ○ Formed on grains
  - ○ Need several 10^4 yr at 20–40 K
  - ○ Possible in our model
- Second generation
  - ○ Formed in warm gas (hot core)
  - ○ Need several 10^3 yr at >100 K
  - ○ Does not occur in our model
- Material in planet-forming zone (5–30 AU) probably abundant in complex organics
  - ○ Spatial variations are likely
- Calculations underway to say more about this

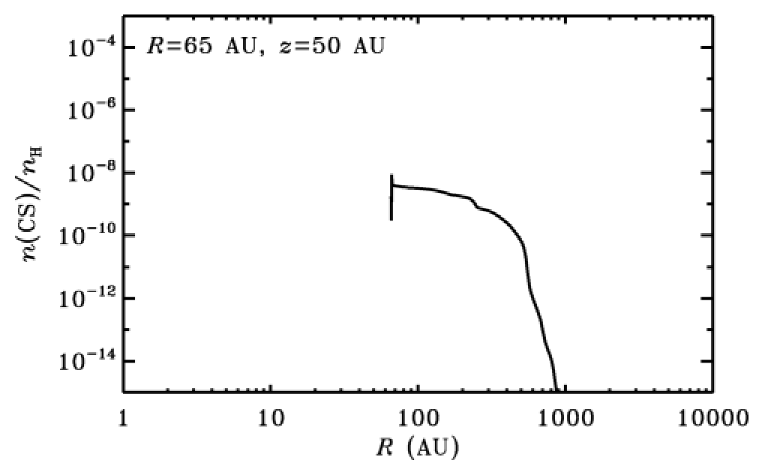
Garrod et al. 2006, 2008

Abundance as function of radius (and time)

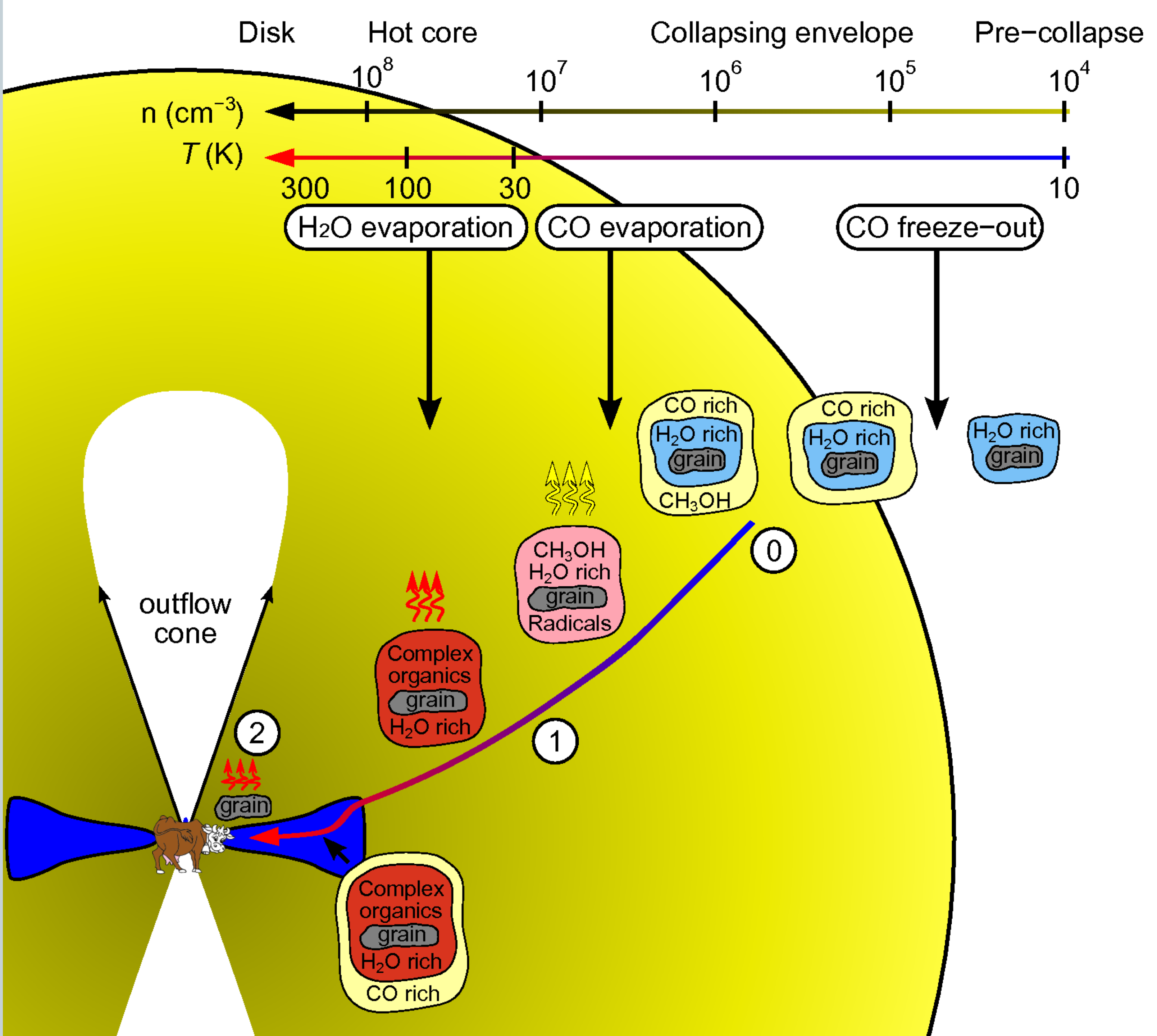








Low-mass star formation



Evolution of gas and dust

Oxygen isotopes in meteorites

- Stability at low temperature:

$$\mathrm{Si^{18}O_4 > Si^{17}O_4 > Si^{16}O_4}$$

- Isotope enhancement (typically a few %):

$$\varepsilon({}^{y}\mathrm{O}) = \frac{([{}^{y}\mathrm{O}]/[{}^{16}\mathrm{O}])_{\mathrm{silicate}}}{([{}^{y}\mathrm{O}]/[{}^{16}\mathrm{O}])_{\mathrm{elemental}}} \qquad (y=17 \text{ or } 18)$$

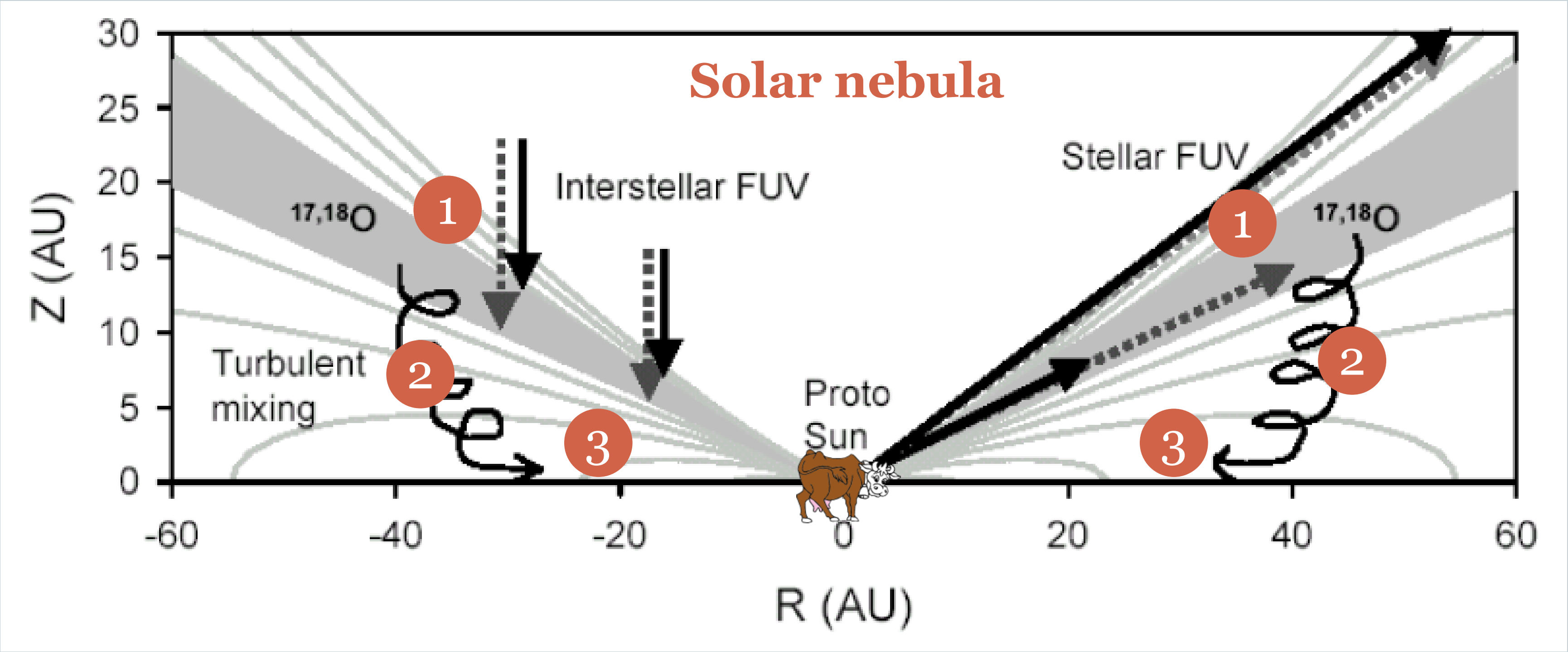
- Expected in meteorites (Matsuhisa et al. 1978):

$$\varepsilon({}^{17}\mathrm{O}) = (0.52 \pm 0.01)\ \varepsilon({}^{18}\mathrm{O})$$

- Measured (Clayton et al. 1973):

$$\varepsilon({}^{17}\mathrm{O}) = (1.0 \pm 0.1)\ \varepsilon({}^{18}\mathrm{O})$$

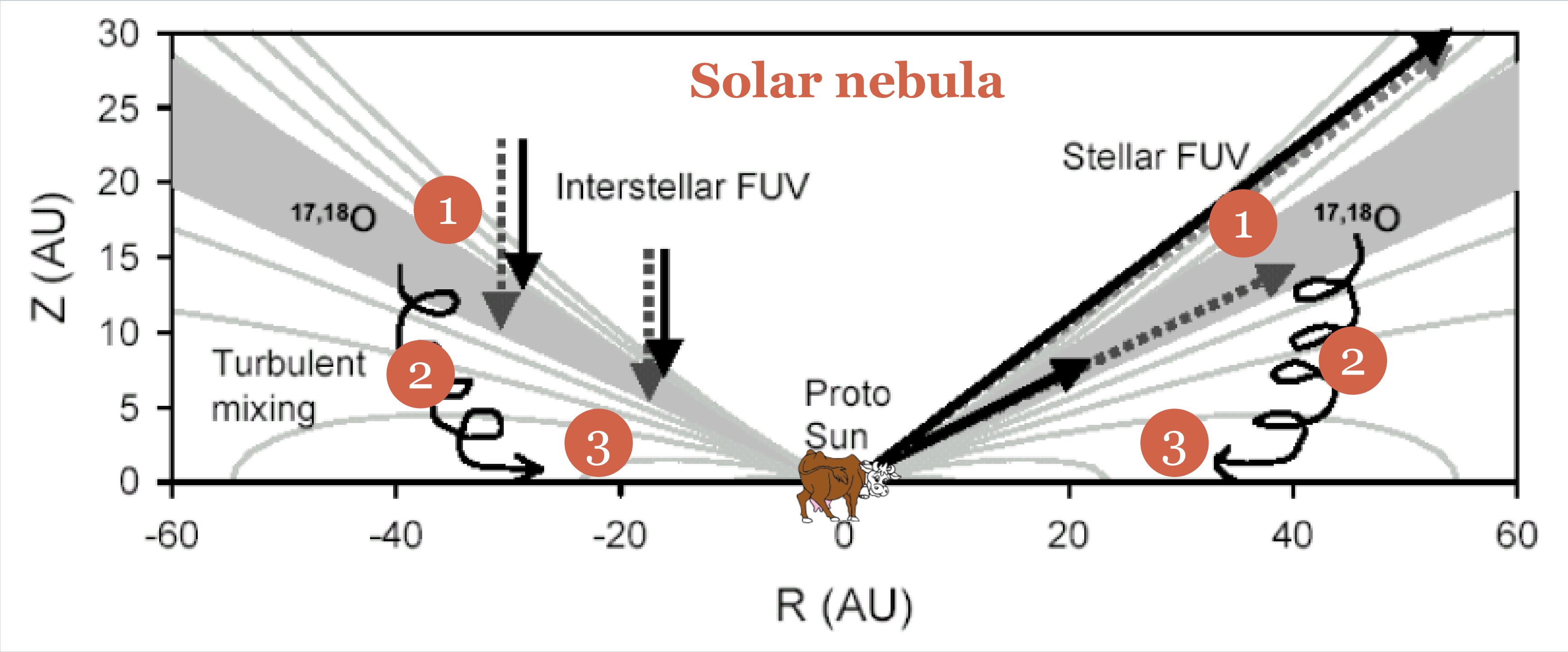
Origin of the isotope anomaly?



1. $C^{17}O$, $C^{18}O$ dissociate faster than $C^{16}O$
2. Enhanced ^{17}O, ^{18}O transported down from surface
3. Enhanced ^{17}O, ^{18}O incorporated into meteoroids

Lyons & Young 2005

Origin of the isotope anomaly?

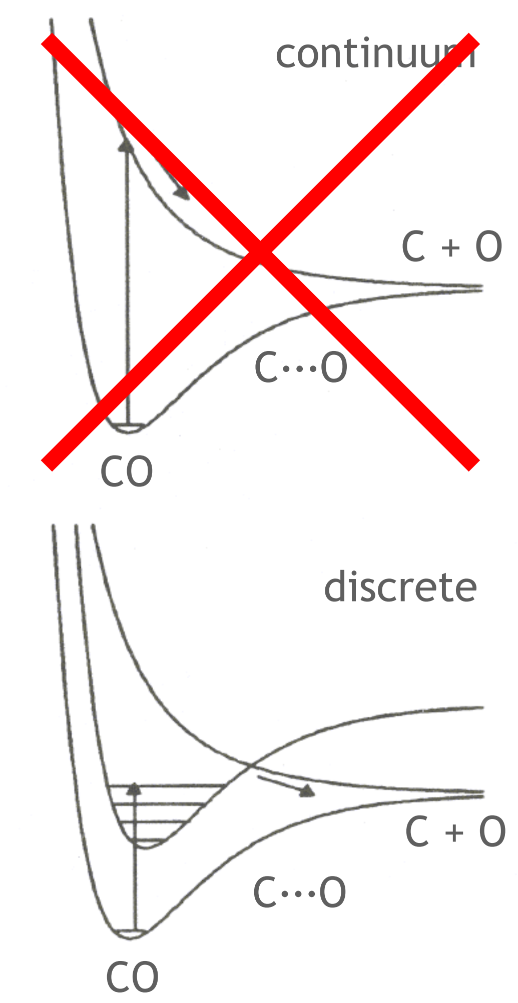


Untested assumption:

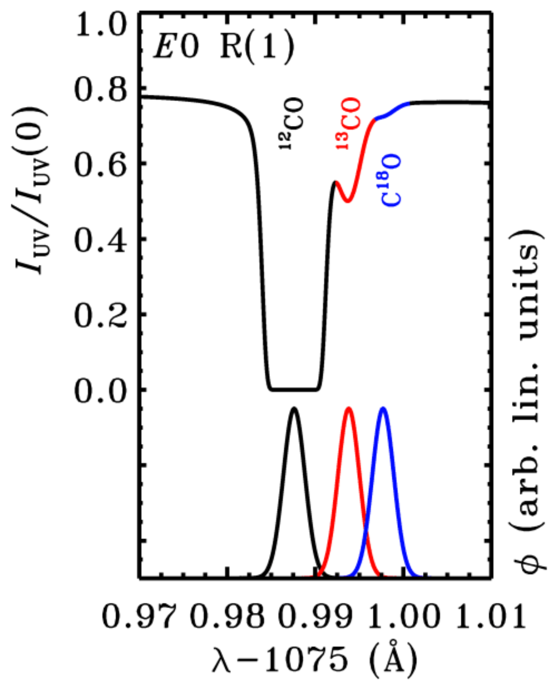
$C^{17}O$ dissociates at same rate as $C^{18}O$

Lyons & Young 2005

CO photodissociation



- 911.75 < λ < 1117.80 Å (13.6 > $h\nu$ > 11.09 eV)
- Discrete transitions only
- Subject to self-shielding



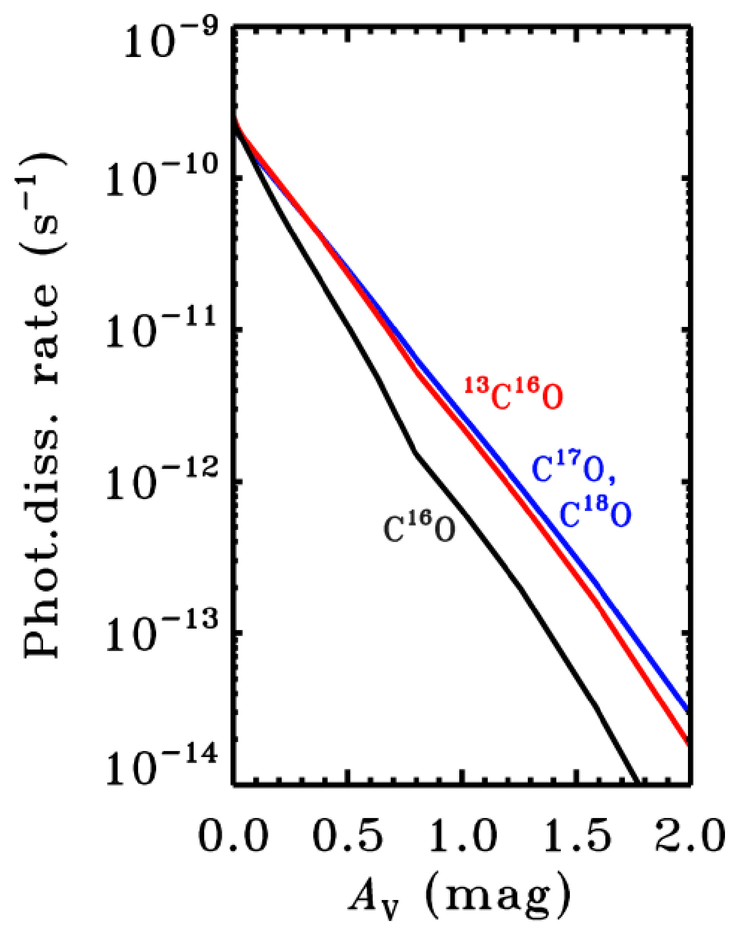
Self-shielding:
- ^{12}CO full
- ^{13}CO, C^{18}O partial
- C^{17}O, ^{13}C^{17}O, ^{13}C^{18}O not

Phot.diss. rate:
- ^{12}CO low
- ^{13}CO, C^{17}O, C^{18}O medium
- ^{13}C^{17}O, ^{13}C^{18}O high

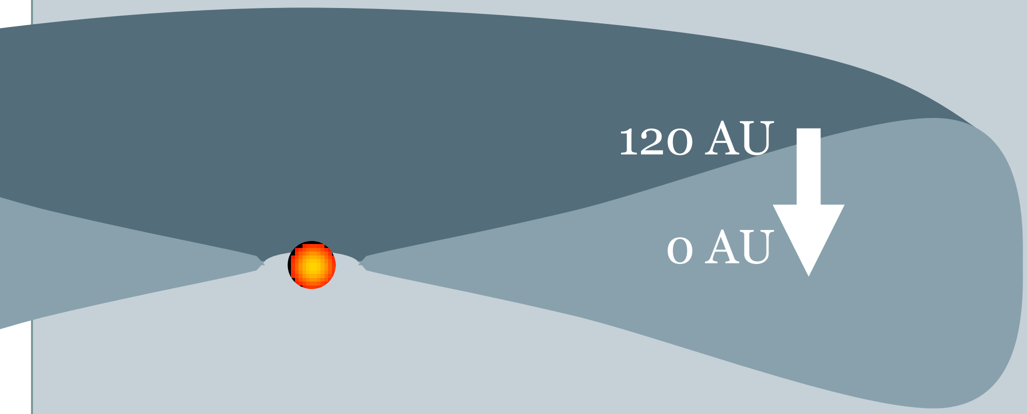
UV photodissociation model

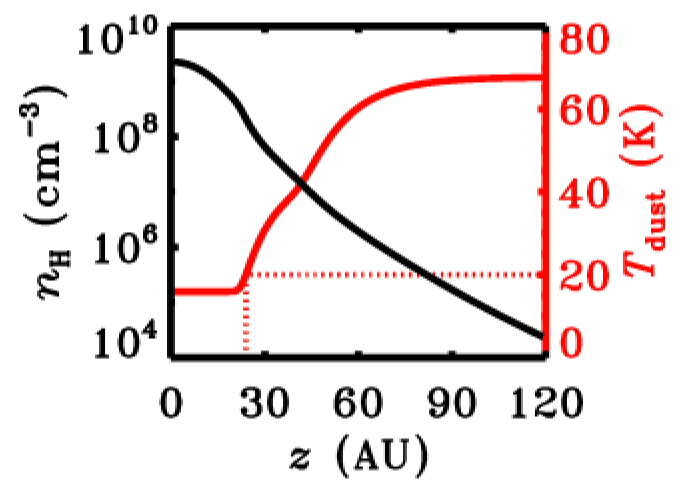
- Same method as van Dishoeck & Black (1988)
- 37 electronic transitions, 5000 individual lines
    - wavelength, oscillator strength, Einstein A from lab data
- Include H/H_2 lines and dust shielding
- Synthesize absorption spectrum for each isotopologue
- Integrate over UV radiation field (Draine, blackbody, …) to get photodissociation rate

Unshielded ISM rate: 2.6×10^{-10} s^{-1}
(30% higher than previous models)



Circumstellar disk model (1)

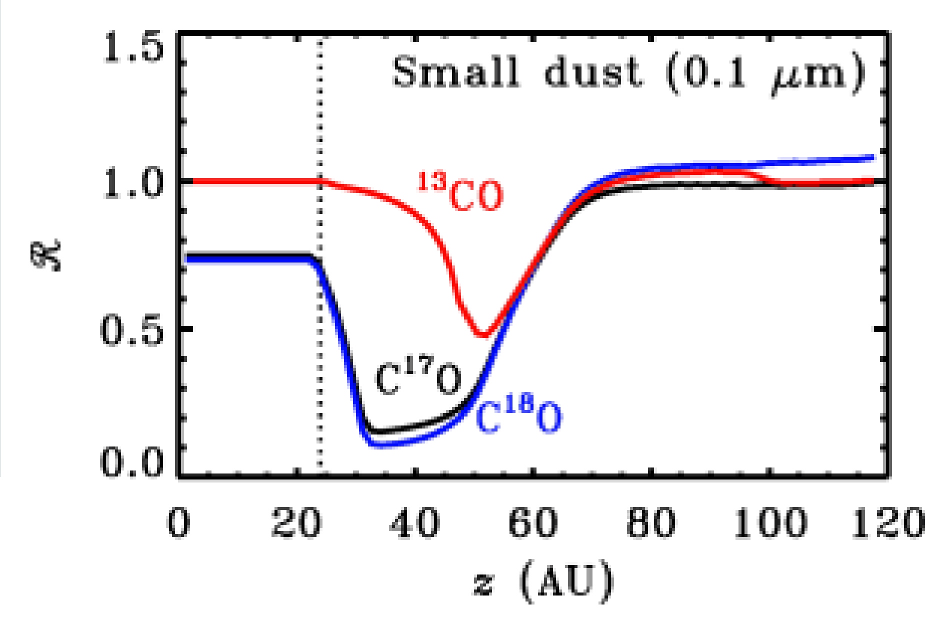




- Vertical cut at r = 105 AU
- CO freezes out below z = 24 AU (T_{dust} = 20 K)
- Normalized column density ratio:

$$R_i(z) = \frac{N_z({}^{x}\mathrm{C}{}^{y}\mathrm{O})}{N_z(\mathrm{C}^{16}\mathrm{O})}\,\frac{[{}^{12}\mathrm{C}]}{[{}^{x}\mathrm{C}]}\,\frac{[{}^{16}\mathrm{O}]}{[{}^{y}\mathrm{O}]}$$

Circumstellar disk model (2)



- ^{13}CO, $C^{17}O$, $C^{18}O$, $^{13}C^{17}O$, $^{13}C^{18}O$ all reduced w.r.t. $C^{16}O$
- Low-T chemistry replenishes some $^{13}C^{16}O$
- ^{17}O and ^{18}O are equally fractionated [$\varepsilon(^{18}O) = \varepsilon(^{17}O)$]

Conclusions

- Gas/ice ratios change during collapse:
  - CO ice desorbs during infall, re-adsorbs in disk below 18 K
  - H_2O ice remains solid, except within a few AU
- Only outer part of disk contains chemically pristine material
- New CO photodissociation rate 30% higher than in previous models
- $C^{17}O$ dissociates at same rate as $C^{18}O$
  - Confirms Lyons & Young hypothesis for $^{17}O/^{18}O$ ratio in meteorites