

Chemical history of ices in protoplanetary disks: Chemistry in a dynamical model

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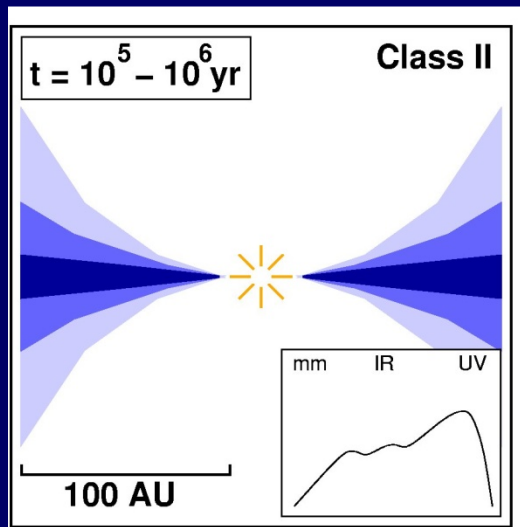
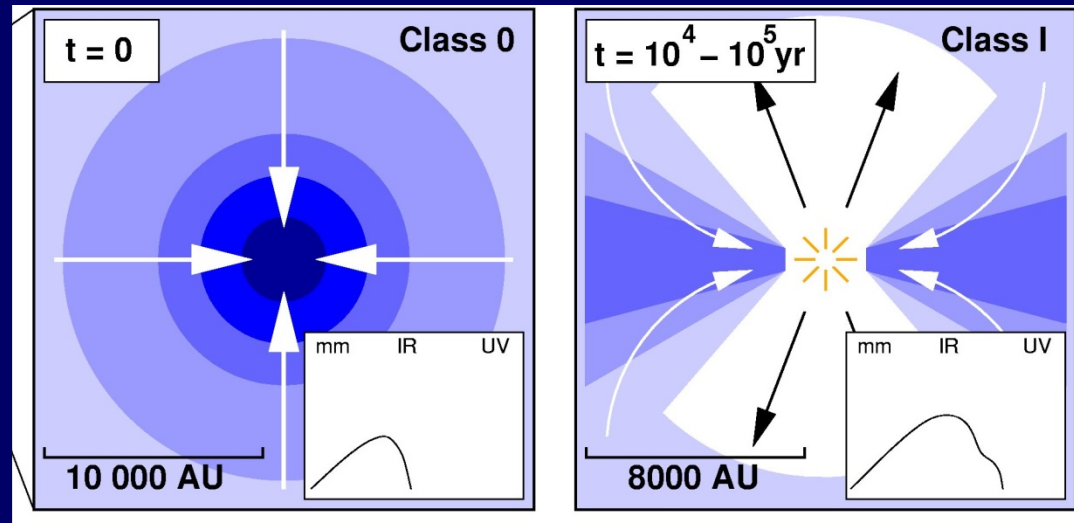
Soon to be in press (A&A)



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)



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

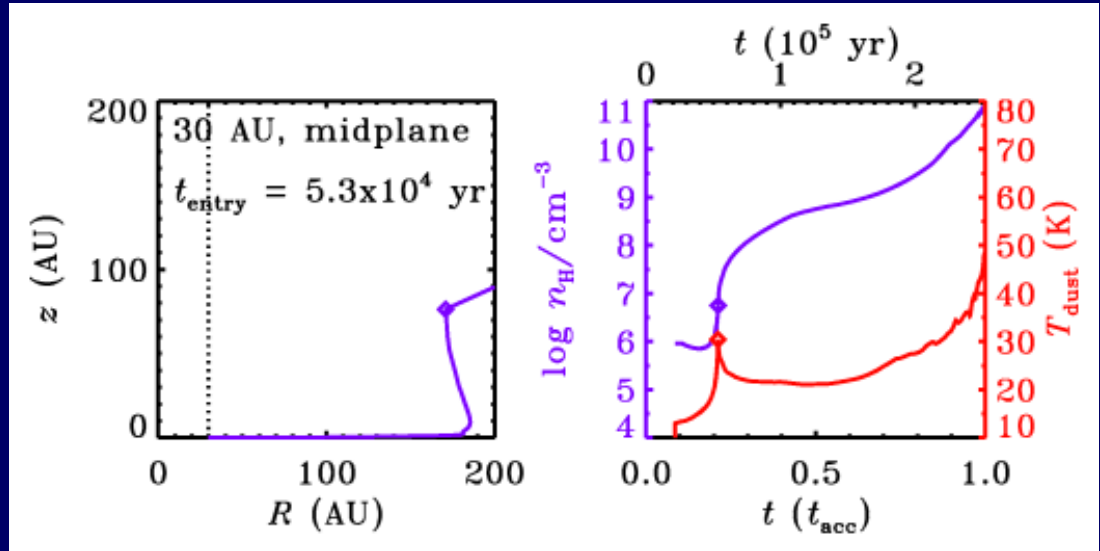
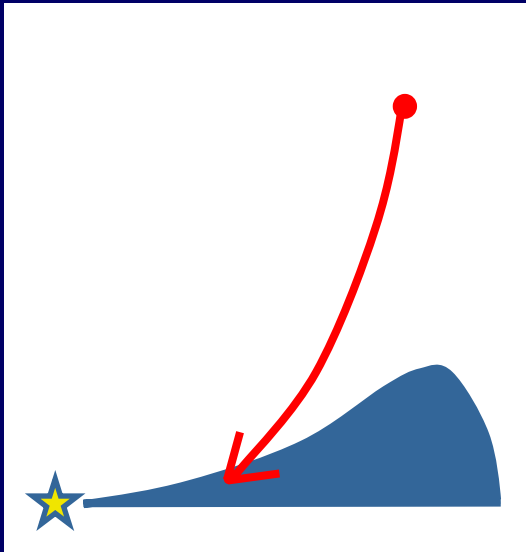
Analytical star formation model

- 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 2008a,b)
- Density profiles compare well with observations
(Jørgensen et al. in prep.)

Easy to change initial conditions

Follow infalling parcels

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

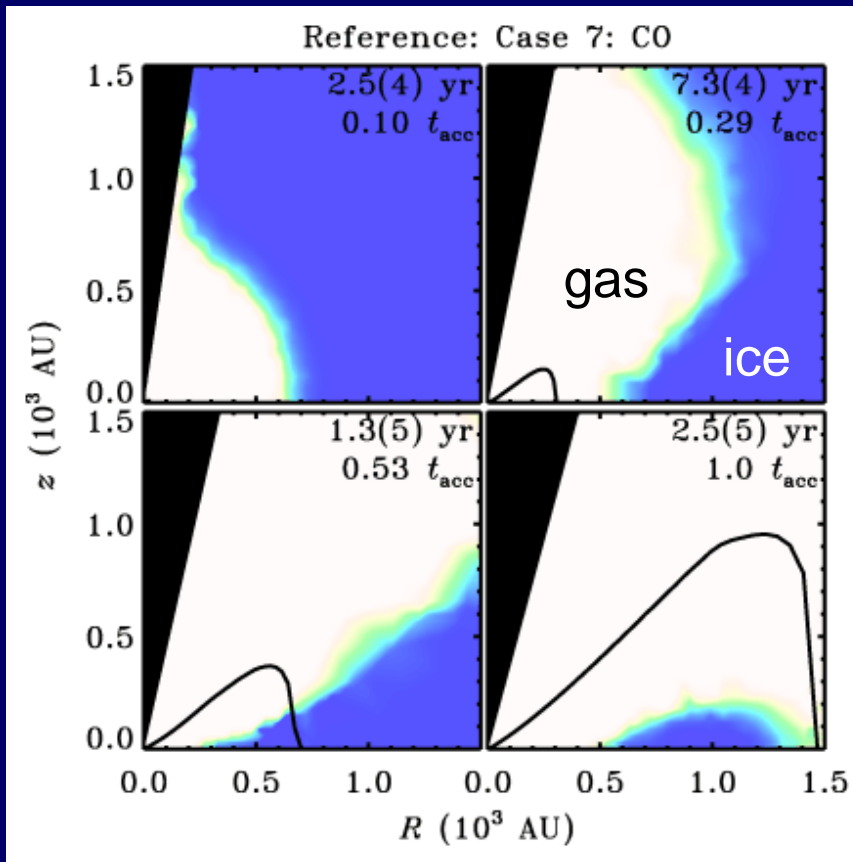


- Jump in n , T upon entering disk
- n increases by factor of $\sim 10^5$ overall, T goes from 10 to several 10s of K

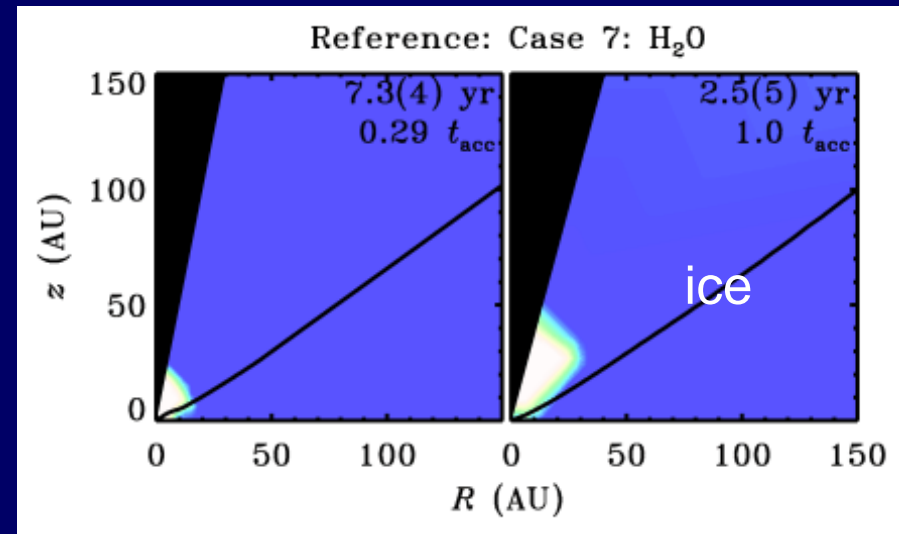
CPU time

- n , v profiles: 5 min
- T_{dust} : 10-60 min for each of 25 time steps
- Trajectories: 30 min for 12,000 parcels
- Gas/ice: 5 s per parcel
(full gas chemistry: 1-10 min per parcel)
- Altogether: 2 days per set of initial conditions, with T_{dust} and gas/ice parallelised

Gas & ice: pure CO, H₂O



CO



H₂O

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

- CO desorbs during infall, re-adsorbs in disk below 18 K
- H₂O remains solid except inner ~10 AU
- Results agree well with numerical simulations

Change initial conditions

- Lower sound speed:
 - Slower accretion, larger and colder disk, more ice
- Lower rotation rate:
 - Less flattening, smaller and warmer disk, less ice
- Lower initial mass:
 - Smaller and slightly colder disk, more ice

Scanning parameter space takes much longer in numerical models

Photodissociation of CO

- Six isotopologues:
 $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, $^{13}\text{C}^{18}\text{O}$
- Dissociation through discrete lines
- Self-shielding at $\sim 10^{15} \text{ cm}^{-2}$
- Isotope-selective: leads to fractionation
- Relevant in wide range of objects:
clouds, PDRs, disks, ...

van Dishoeck & Black (1988)

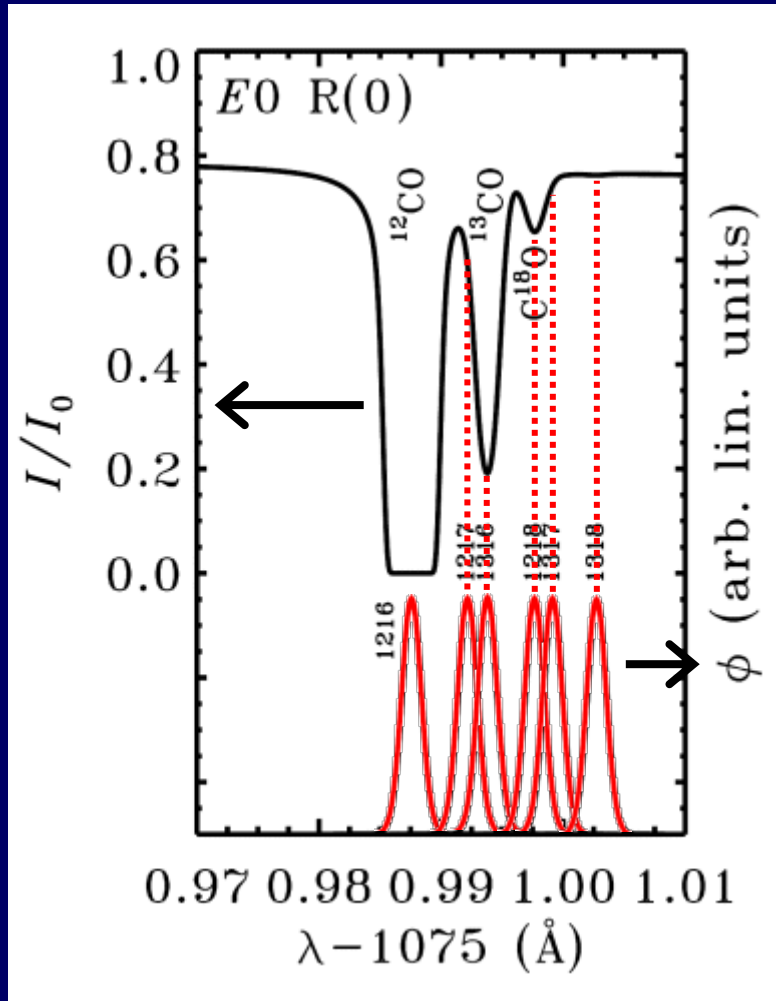
- Detailed line model
- Limited spectroscopic data
- No $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$
- Low excitation temperatures only
- Shielding functions
- Couple to chemical network

New model

- New molecular data
 - Line positions, identifications
 - Oscillator strengths
 - Lifetimes, predissociation probabilities
 - Rotational constants
- All six isotopologues
- Include higher excitation temperatures

- Old rate in ISM: $2.0 \times 10^{-10} \text{ s}^{-1}$
- New rate in ISM: $2.6 \times 10^{-10} \text{ s}^{-1}$

Isotope-selective shielding



$\sim 92930 \text{ cm}^{-1}$

$^{12}\text{C}^{16}\text{O}$

strong shielding

$^{13}\text{C}^{16}\text{O}$

$^{12}\text{C}^{17}\text{O}$

$^{12}\text{C}^{18}\text{O}$

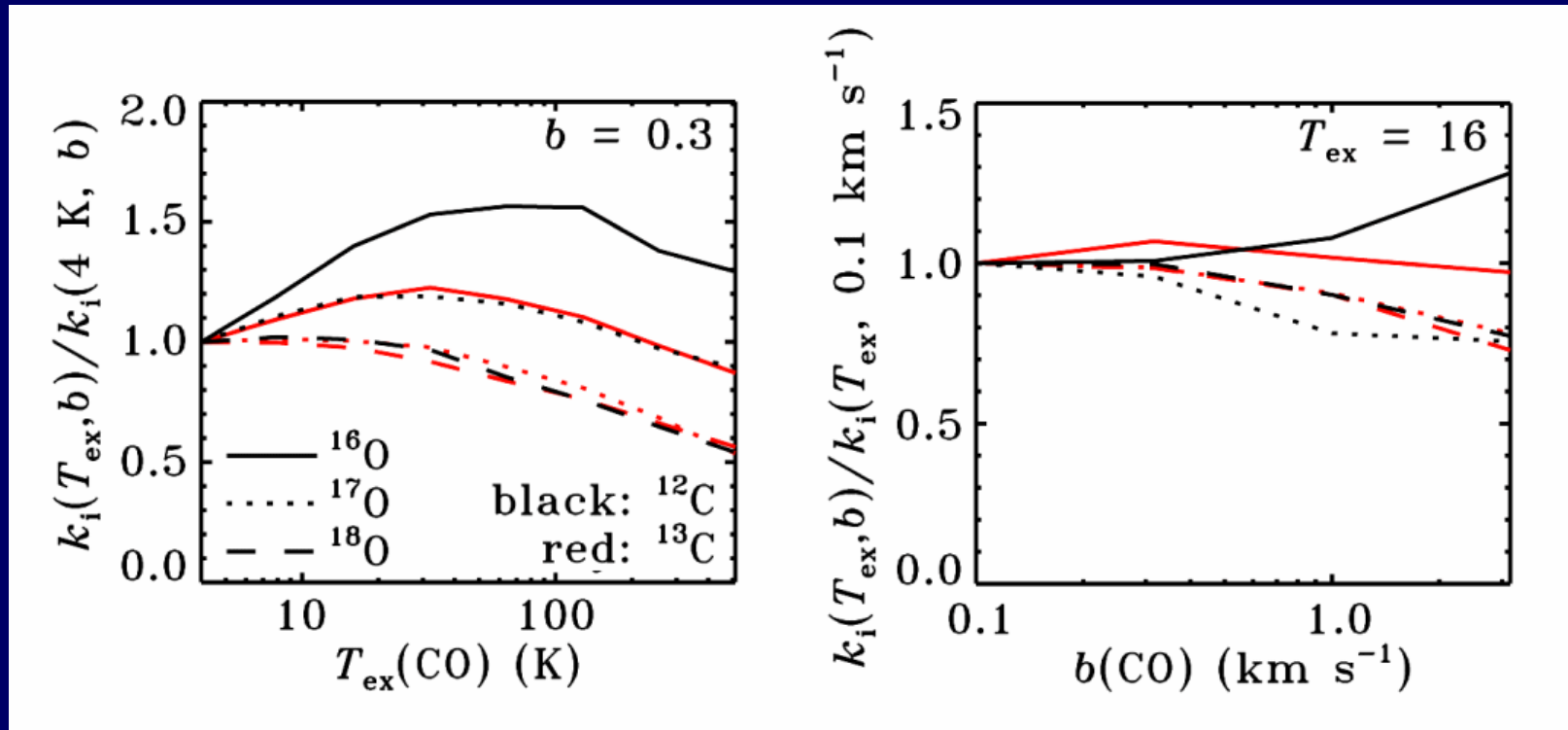
$^{13}\text{C}^{17}\text{O}$

$^{13}\text{C}^{18}\text{O}$

weak shielding

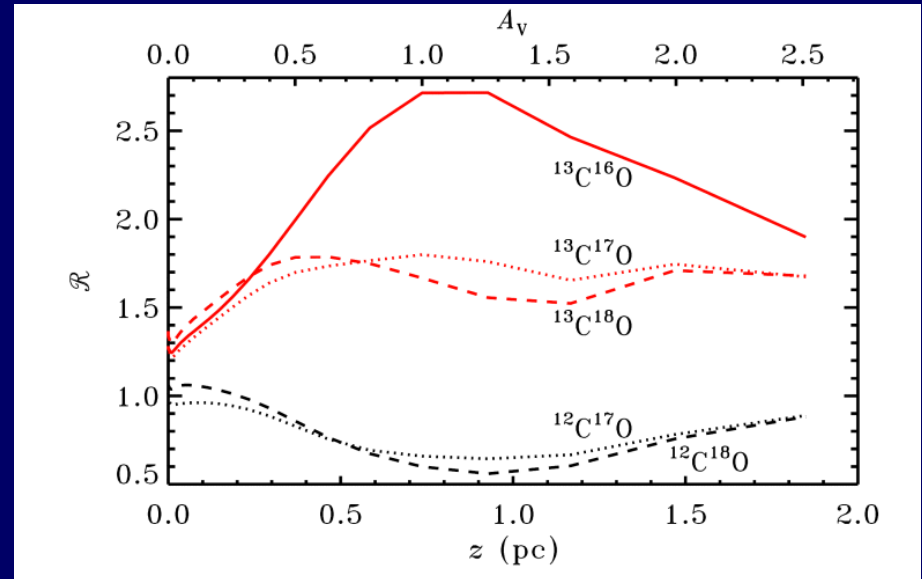
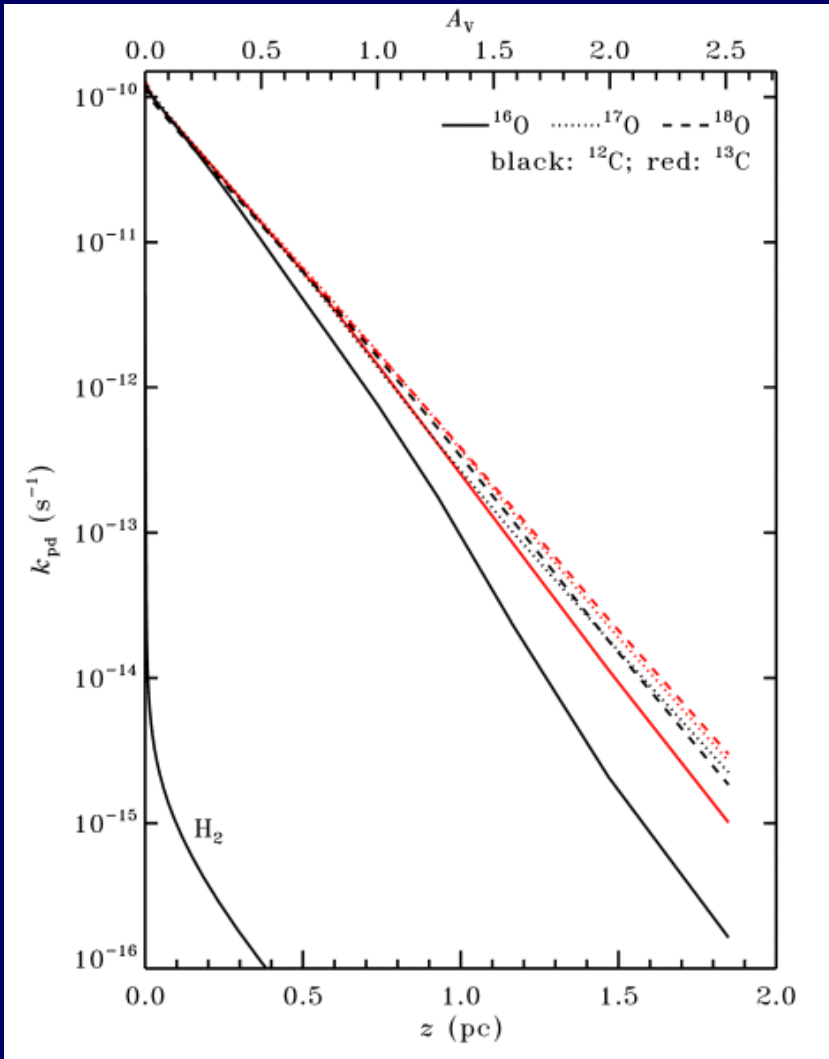


Excitation temperature, Doppler width



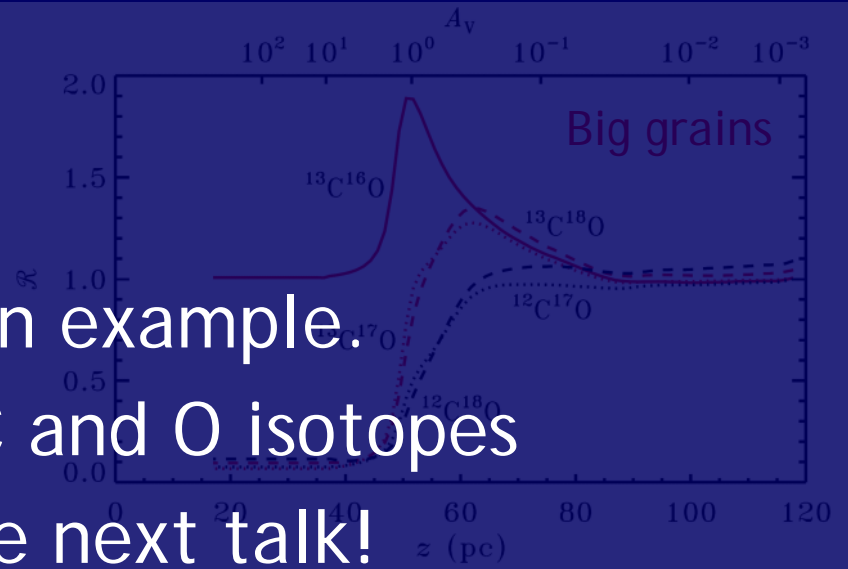
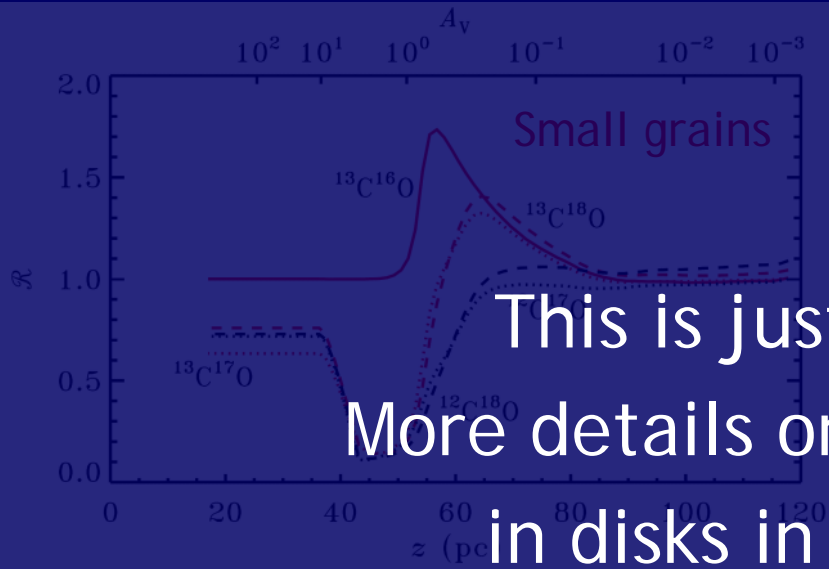
- Higher T_{ex} : less self-shielding, more H_2 shielding
- Higher b : same effect

Translucent cloud



- $n = 700 \text{ cm}^{-3}$, $T = 30 \text{ K}$
- Model includes reactions like $CO + ^{13}C^+ \rightleftharpoons C^+ + ^{13}CO + 35 \text{ K}$
- R is normalized cumulative column density ratio
- ^{13}CO , $^{13}C^{17}O$, $^{13}C^{18}O$ enhanced; $C^{17}O$, $C^{18}O$ reduced

Circumstellar disk



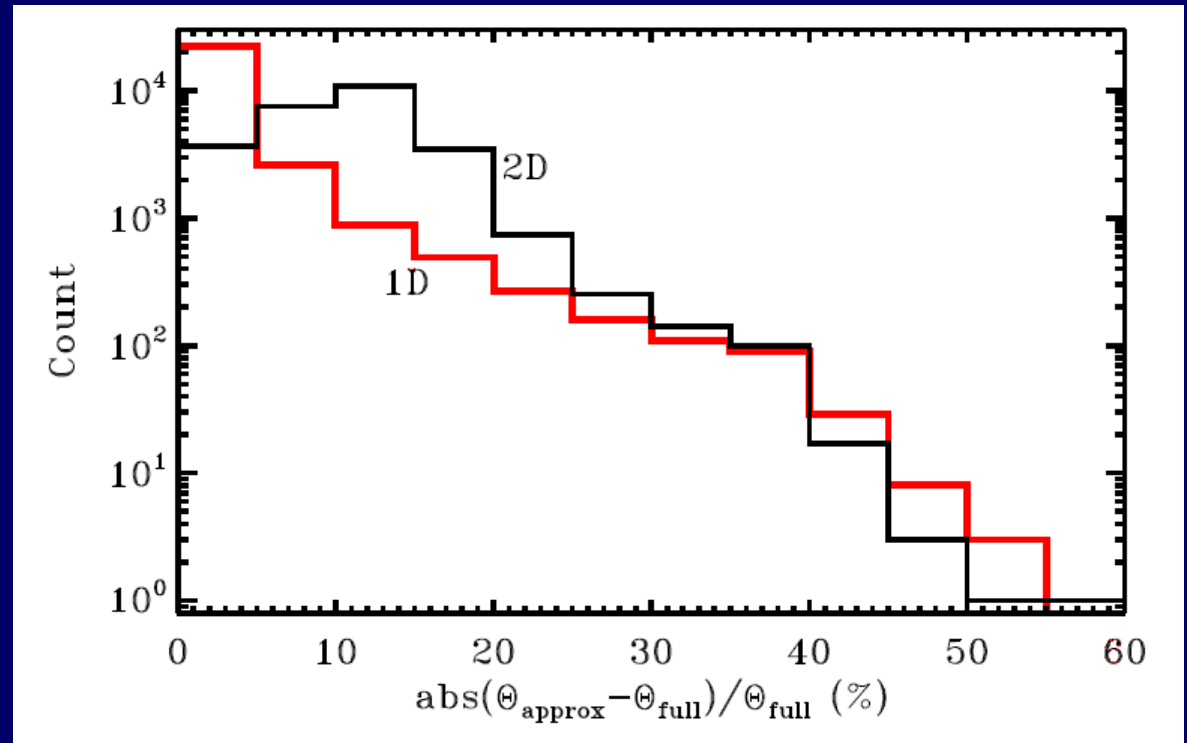
This is just an example.
More details on C and O isotopes
in disks in the next talk!

- Vertical cut at 105 AU
- All isotopologues but ^{13}CO reduced relative to ^{12}CO
- Bigger grains: photodissociation important to larger A_V , R frozen at other values
- CO frozen below 35 AU

^{17}O and ^{18}O equally fractionated:
explains meteoritic ^{18}O anomaly?
(Clayton et al. 1973; Lyons & Young 2005)

Shielding functions

- Pre-computed on 1D or 2D grid of $N(\text{CO})$ and $N(\text{H}_2)$, then interpolate
- Error at most 50% in grid of translucent cloud models
- Full calculation: minutes,
interpolation: seconds



Conclusions

- Gas/ice ratios change during collapse:
 - CO ice desorbs during infall, re-adsorbs in disk below 18 K
 - H₂O remains solid, except within a few AU
- Analytical works as well as numerical, and is much faster
- Invest CPU time where you need it (T_{dust})
- CO photodissociation seems well described by pre-computed shielding functions (but need to confirm with more tests)