Models of fractionation in disks

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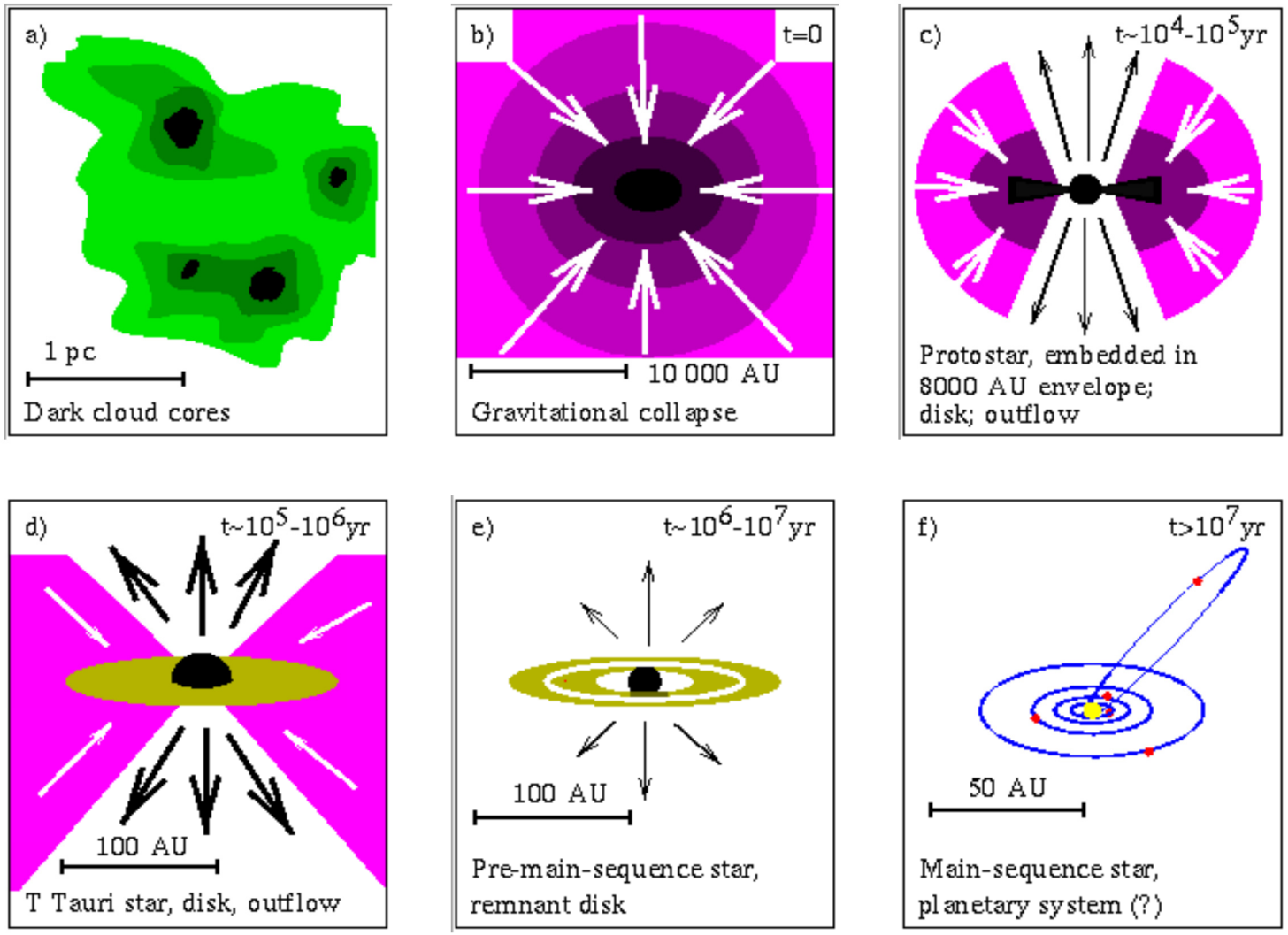
Outline

- Static disk models
  - What processes affect isotope ratios in disks and can they change the ratios inherited from the interstellar medium?
    - Deuterium
- Mixing models (vertical mixing at 5 AU – near Jupiter's orbit)
  - What effect does vertical mixing have on
    - (a) Distribution of molecules between gas and ice
    - (b) Isotope ratios
  - Deuterium
  - Carbon and oxygen

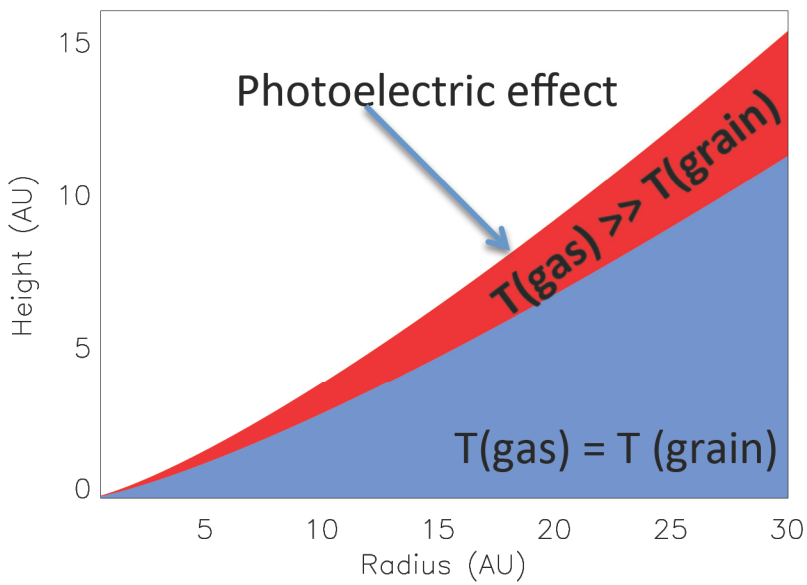
Star formation



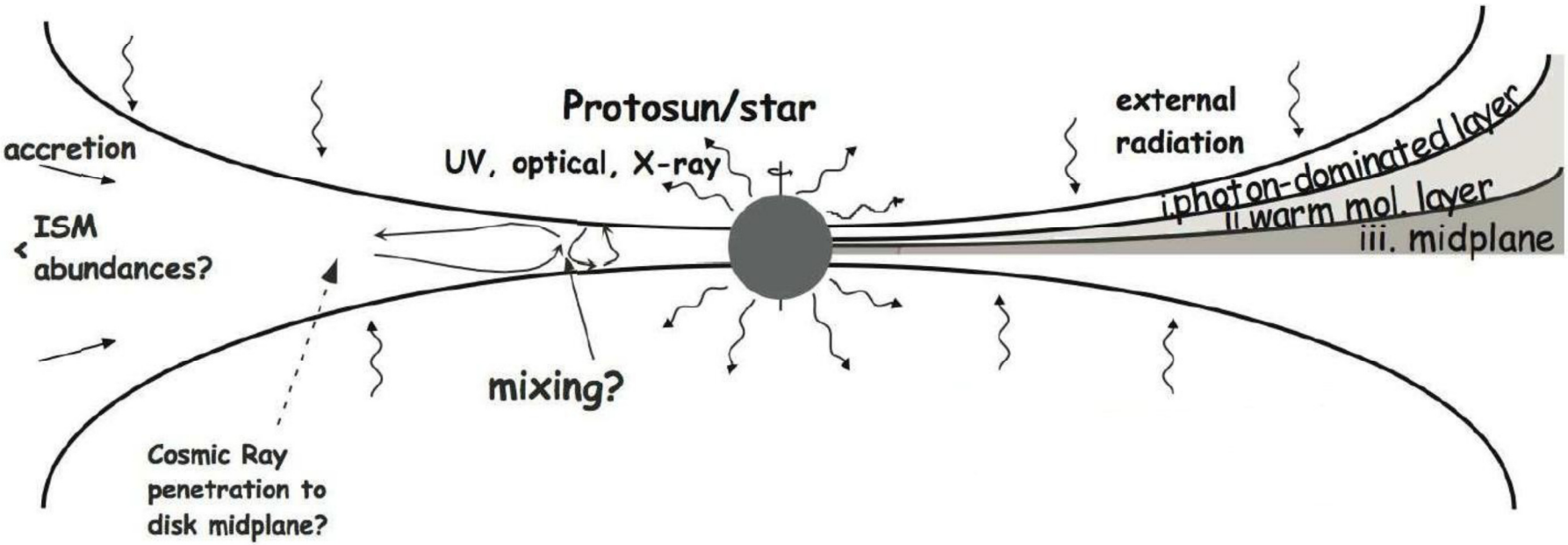
M.Hogerheijde (1998), Shu et al. (1987)

Disk models

- Hydrostatic models (d'Alessio et al.) provide n(R,z), $T_{grain}(R,z)$
- $T_{gas}(R,z)$ from balancing heating and cooling processes (Kamp & Dullemond 2004, Kamp & van Zadelhoff 2001)
- Initial chemical abundances from molecular cloud model
- Basic reaction network from the UMIST database (RATE06: Woodall et al. 2007)
  - Gas phase reactions
  - Irradiation by UV, cosmic rays, X-rays
  - Freezeout and desorption
  - Grain surface reactions



Disk chemistry



Bergin et al. 2007

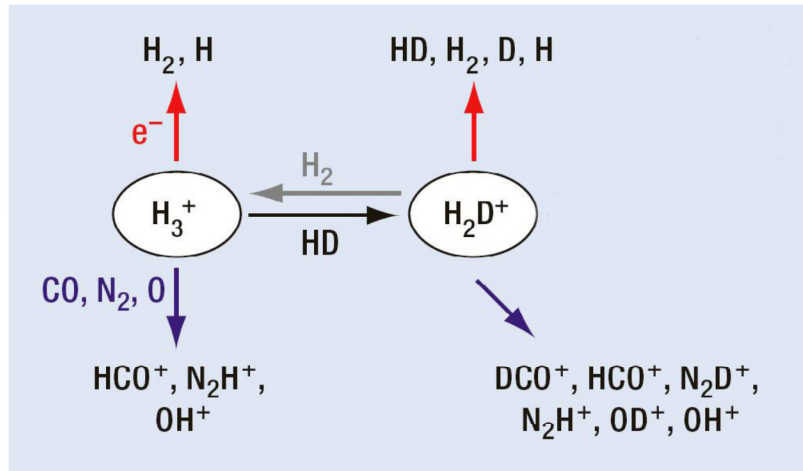
Deuterium fractionation in static disks

What causes fractionation?

- Deuterium
  - Gas phase

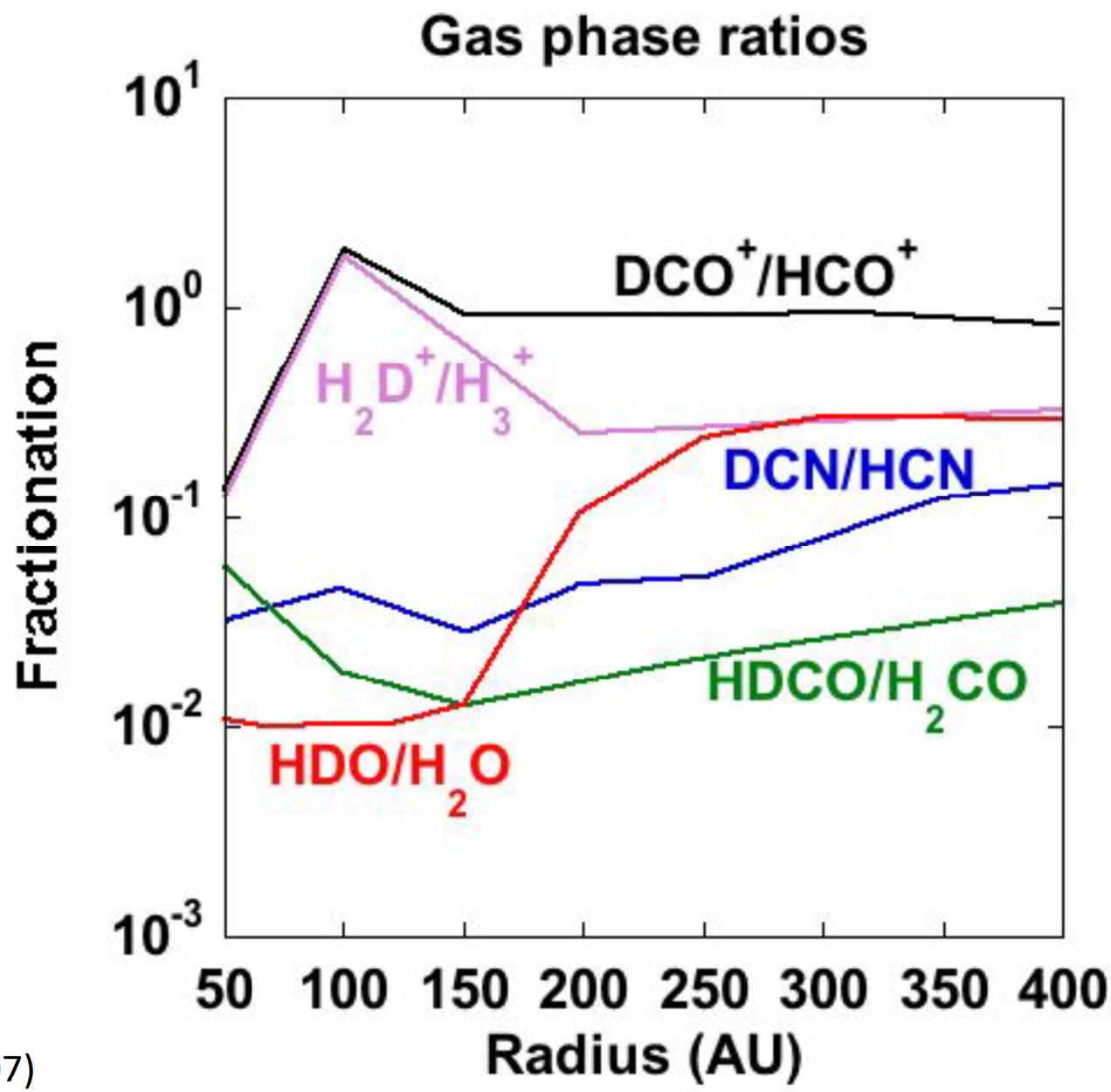
$$H_3^+ + HD \Leftrightarrow H_2D^+ + H_2 + \Delta E = 220K$$
$$CH_3^+ + HD \Leftrightarrow CH_2D^+ + H_2 + \Delta E = 370K$$
$$C_2H_2^+ + HD \Leftrightarrow C_2HD^+ + H_2 + \Delta E = 550K$$

Millar 2005



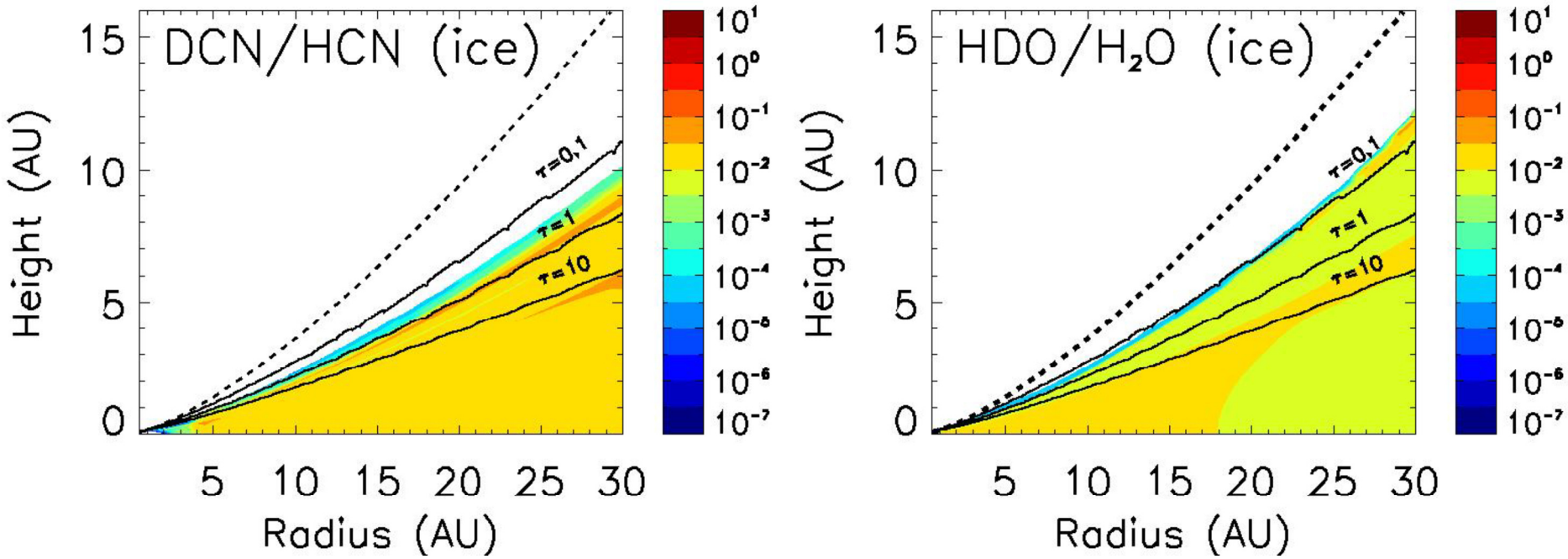
  - Grain chemistry
    - Enhanced D/H atomic ratios on grains leads to high D/H in molecules formed on grains e.g. formaldehyde, water and methanol

- Primordial D/H ratio ≈ 10^{-5}
  - Cold regions molecular D/H ratios can be as high as 0.1



Willacy (2007)

Deuterated ices



Model ratios:

DCN/HCN (ice) = 9.0×10^{-3}

HDO/H_2O (ice) > 10^{-2}

Willacy & Woods (2009)

Comet observations:

x(DCN)/x(HCN) = 2.3×10^{-3}

$x(HDO)/x(H_2O) = 5.0-6.6 \times 10^{-4}$ Oort cloud

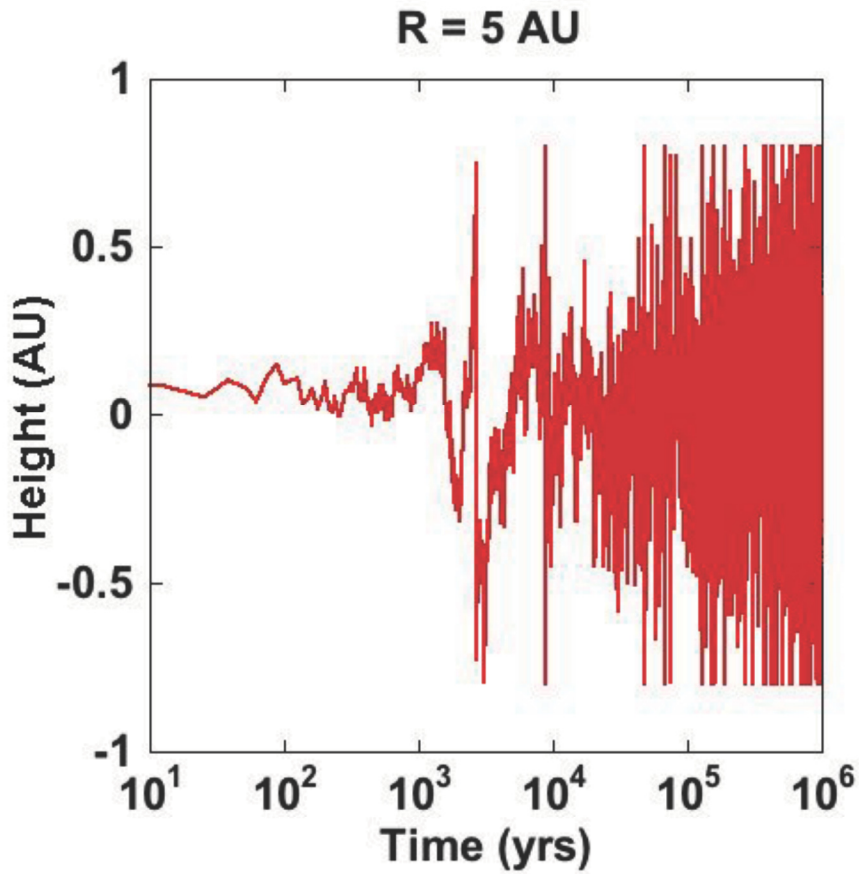
$x(HDO)/x(H_2O) = 1.6 \times 10^{-4}$ Jupiter family

(Hartogh et al. 2011)

Mixing models

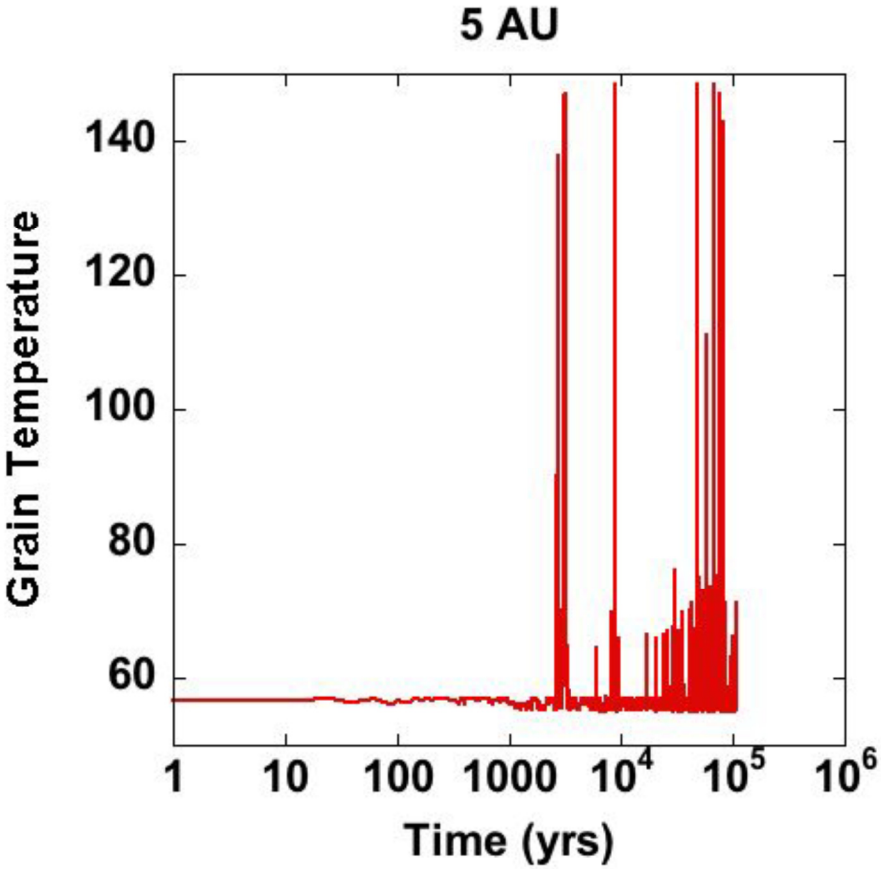
Mixing models

- Trace the vertical motion of a parcel of gas and dust in the disk at 5 AU using 3D MHD code.
- MHD shearing box calculation:
  - 600 particles
  - 300 orbits (Orbital period = 4×10^8 s)
  - take trajectories from 50 – 300 orbits
  - Concatenate trajectories together to make one path covering 1 Myrs
- MHD gives n(t), $T_{gr}(t)$

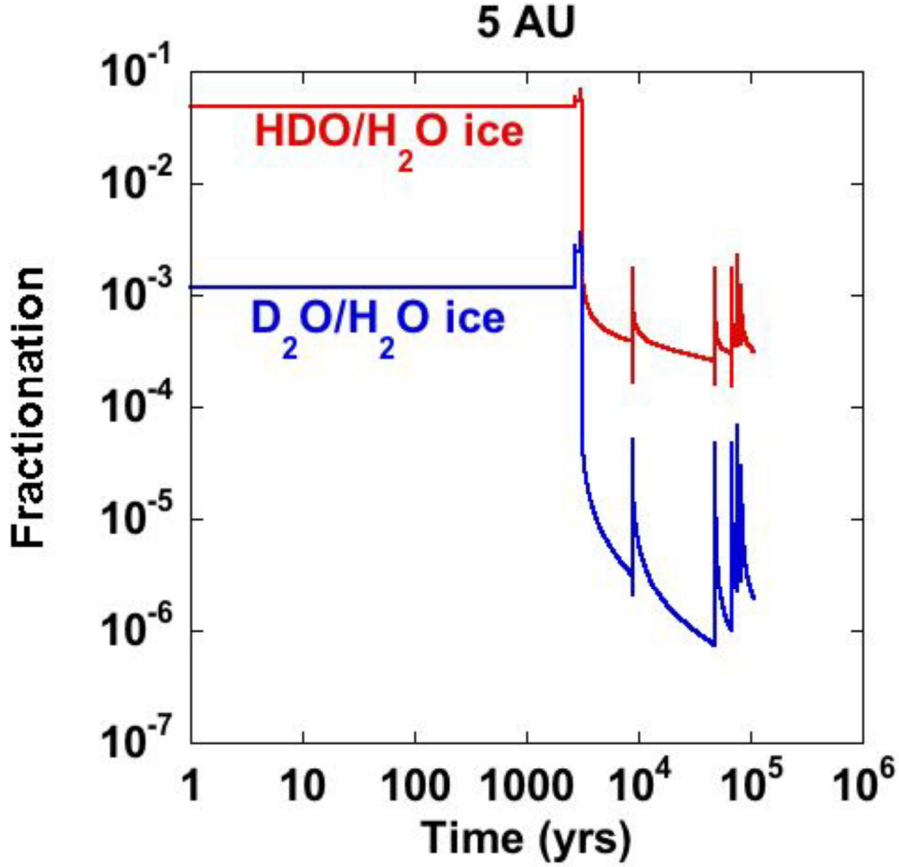


Inputs to chemical model

Grain temperature

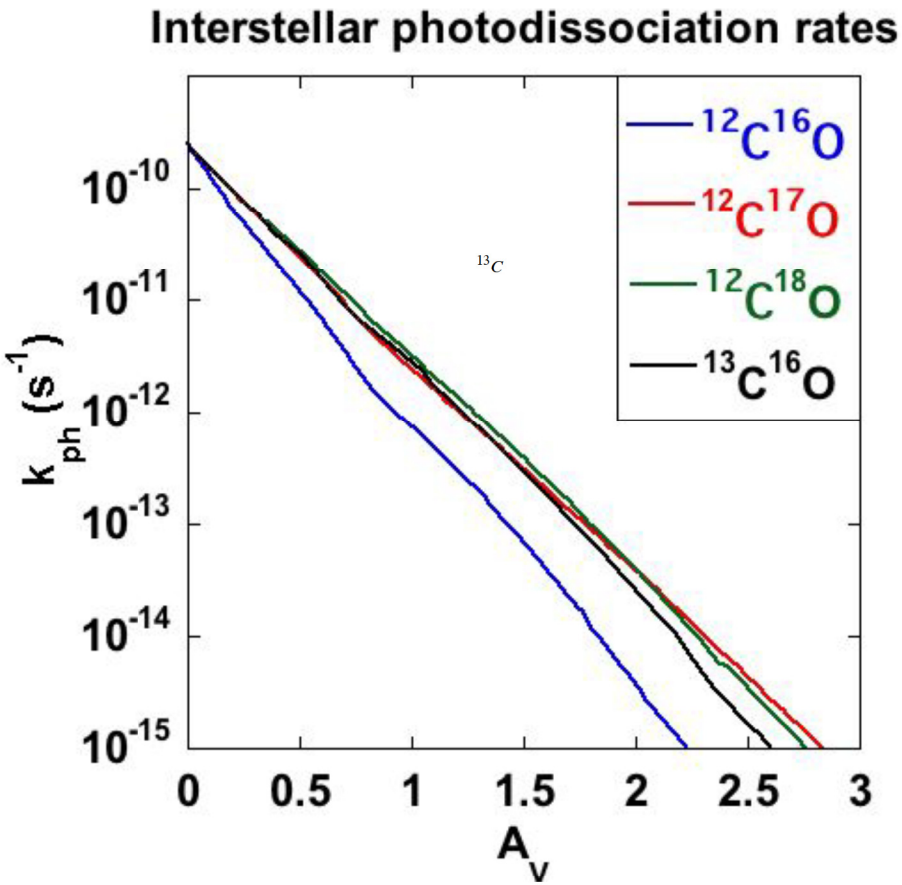


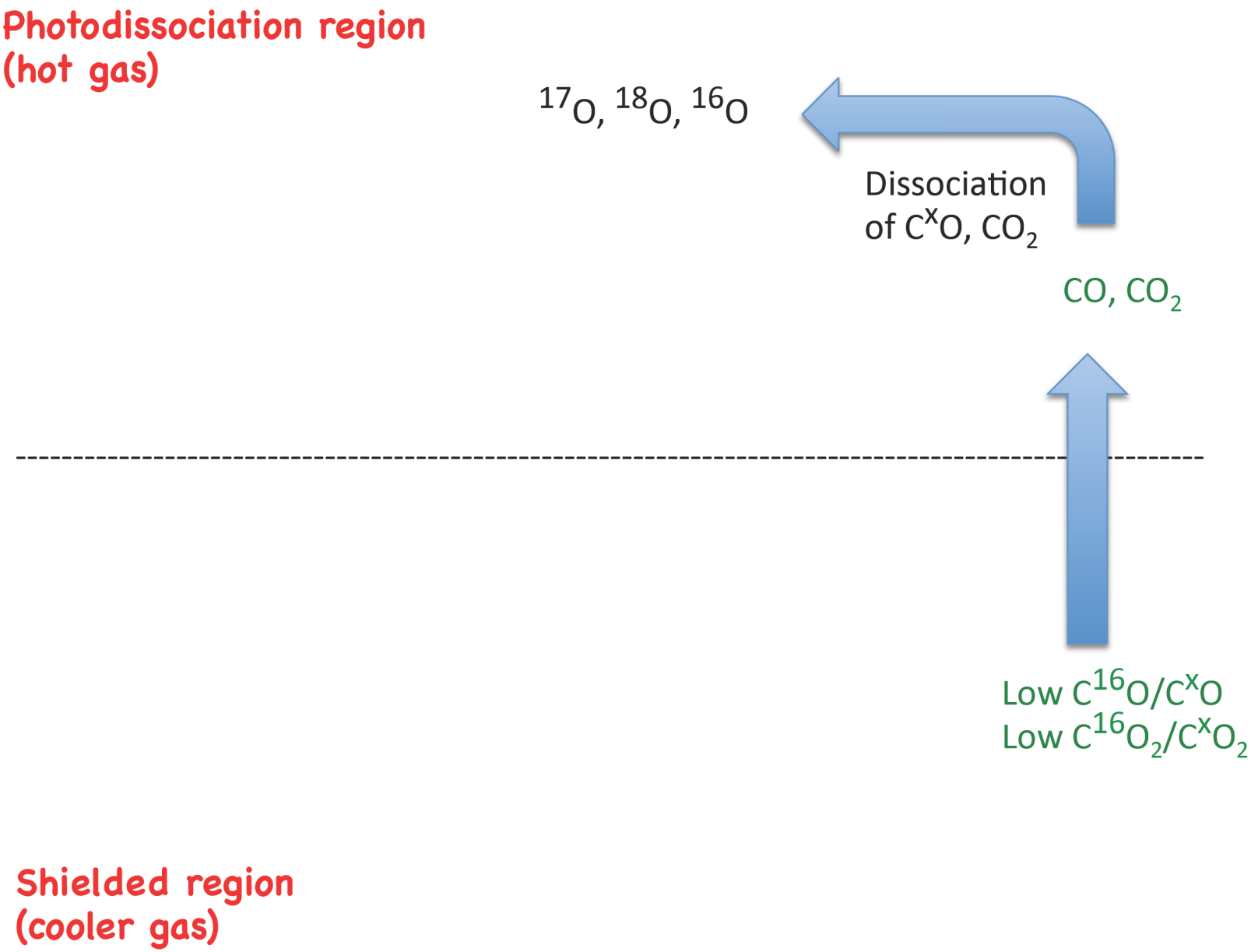
Deuteration of water ice

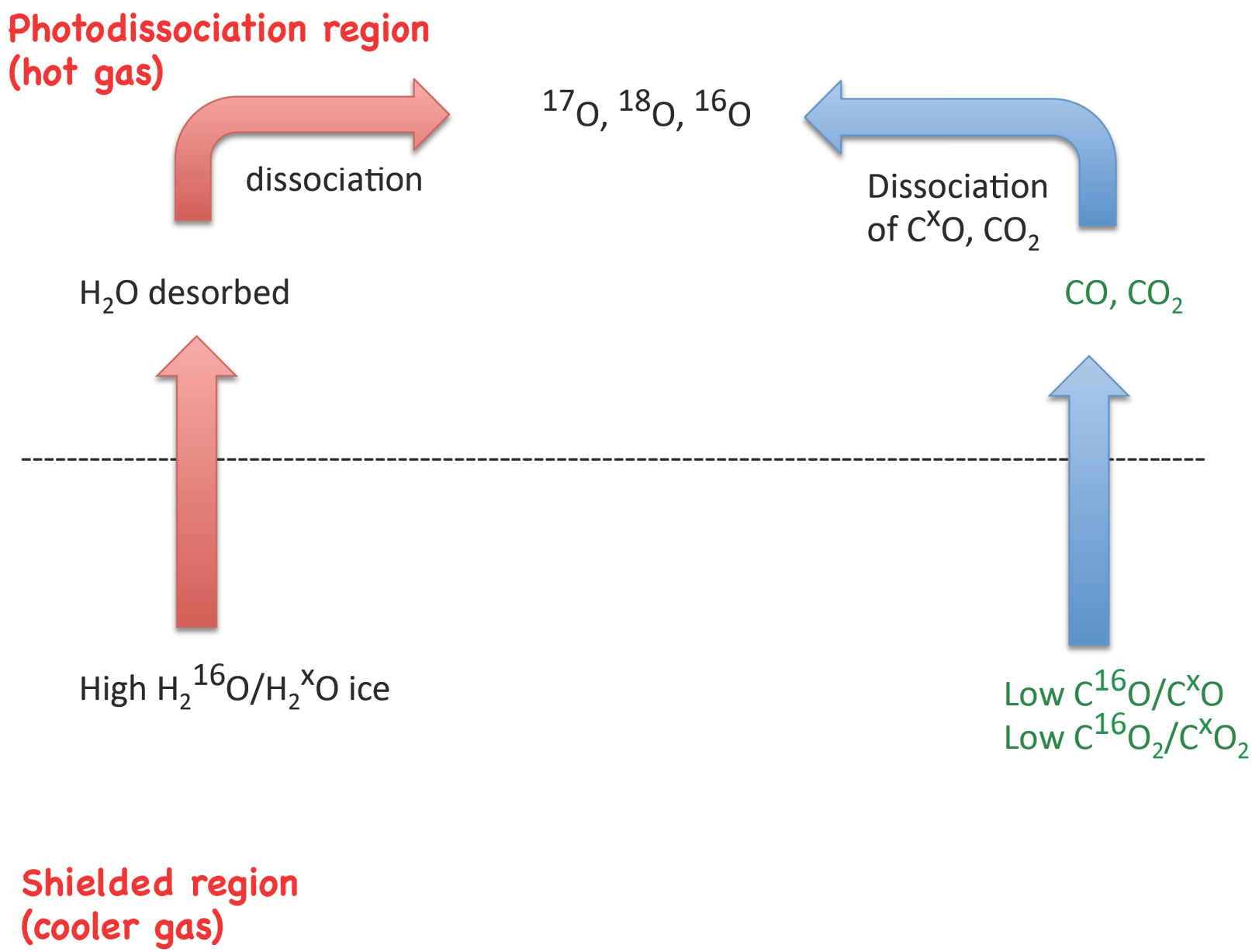


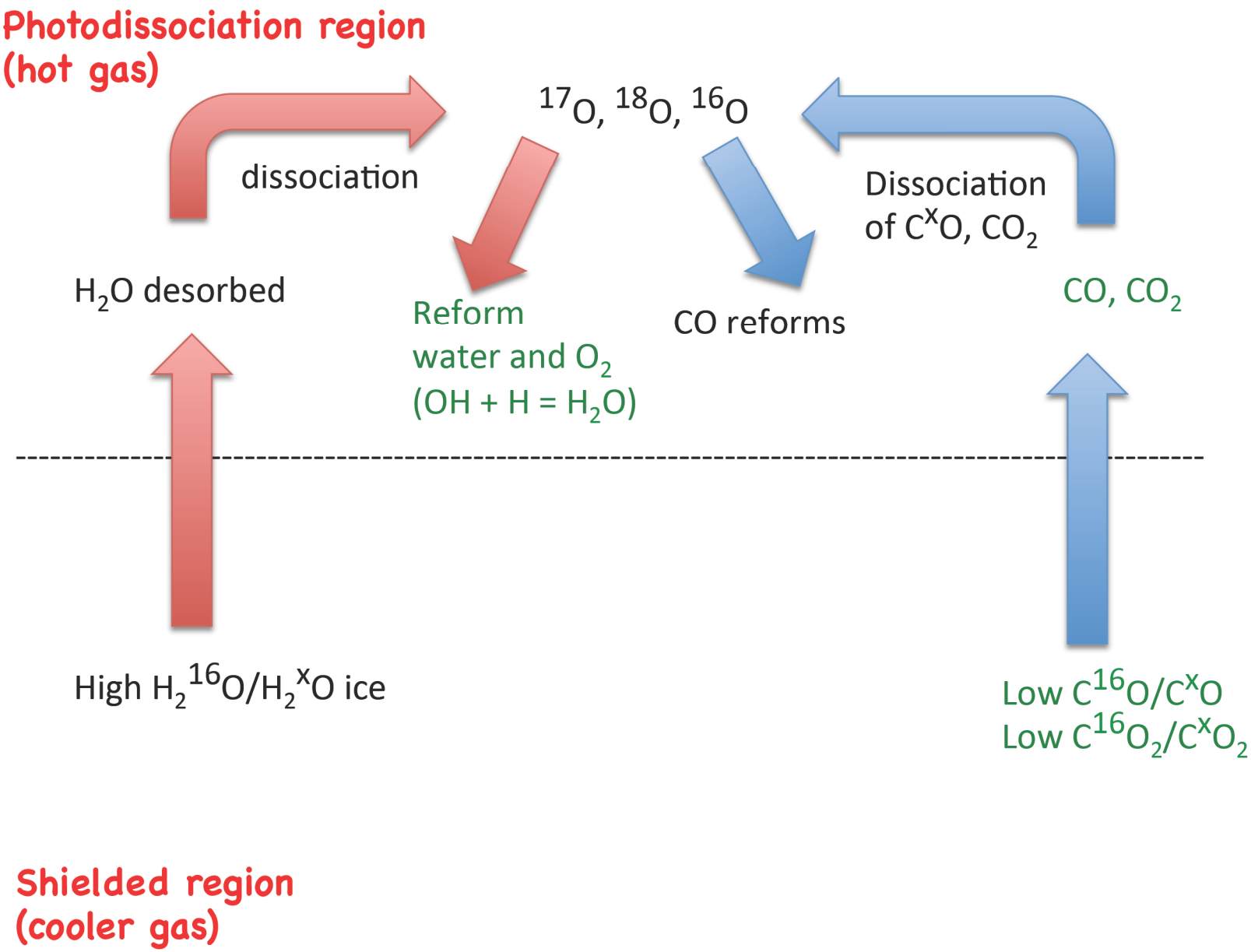
Selective photodissociation of CO

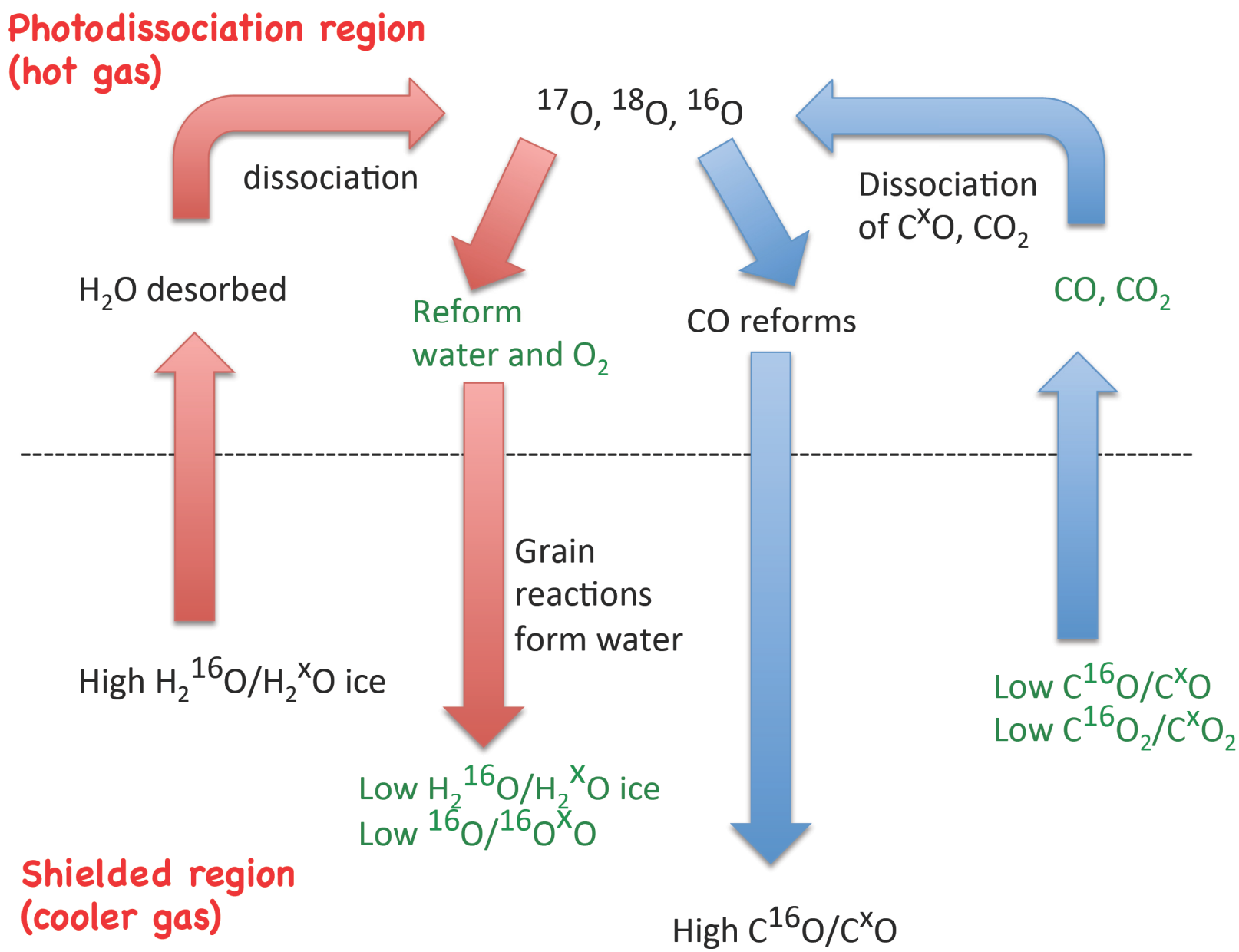
- Rates from Visser et al (2009)



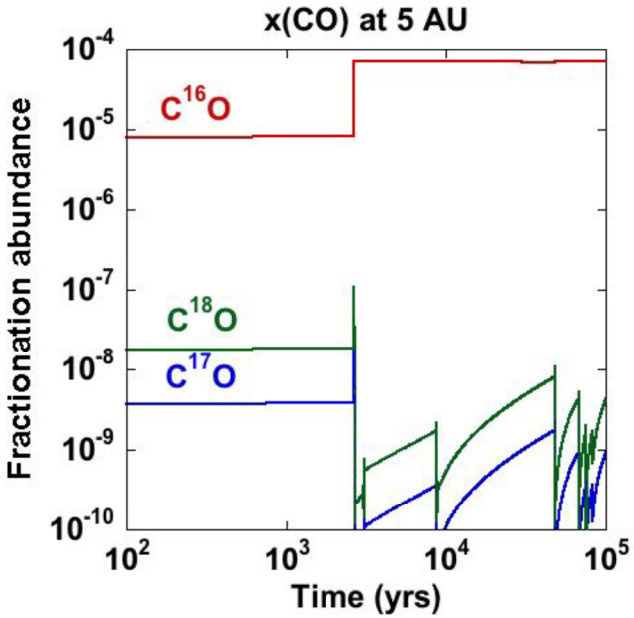

Photodissociation region
(hot gas)
^{17}O, ^{18}O, ^{16}O
Dissociation
of C^xO, CO_2
CO, CO_2
Low $C^{16}O/C^xO$
Low $C^{16}O_2/C^xO_2$
Shielded region
(cooler gas)

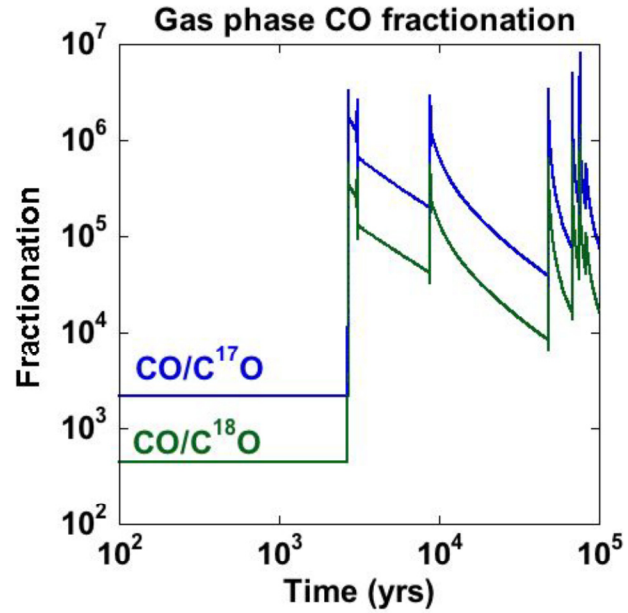

Photodissociation region
(hot gas)
dissociation
^{17}O, ^{18}O, ^{16}O
Dissociation
of C^xO, CO_2
H_2O desorbed
CO, CO_2
High $H_2{}^{16}O/H_2{}^xO$ ice
Low $C^{16}O/C^xO$
Low $C^{16}O_2/C^xO_2$
Shielded region
(cooler gas)

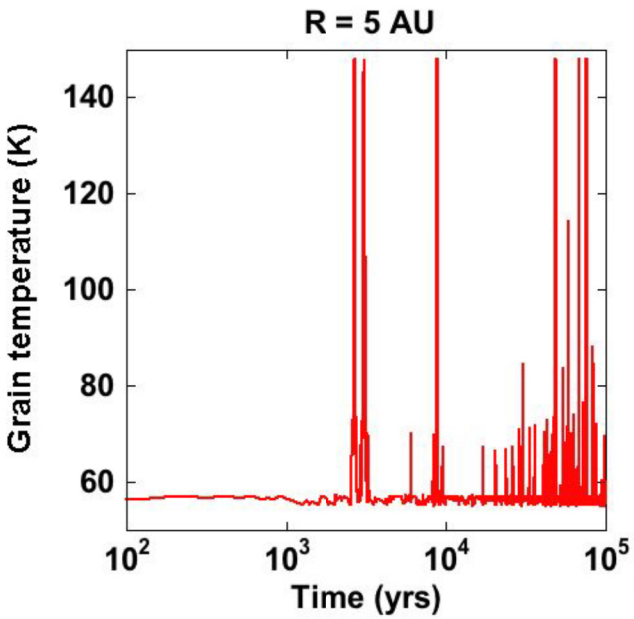

Photodissociation region
(hot gas)
^{17}O, ^{18}O, ^{16}O
dissociation
Dissociation
of C^xO, CO_2
H_2O desorbed
Reform
water and O_2
($OH + H = H_2O$)
CO reforms
CO, CO_2
High $H_2{}^{16}O/H_2{}^xO$ ice
Low $C^{16}O/C^xO$
Low $C^{16}O_2/C^xO_2$
Shielded region
(cooler gas)

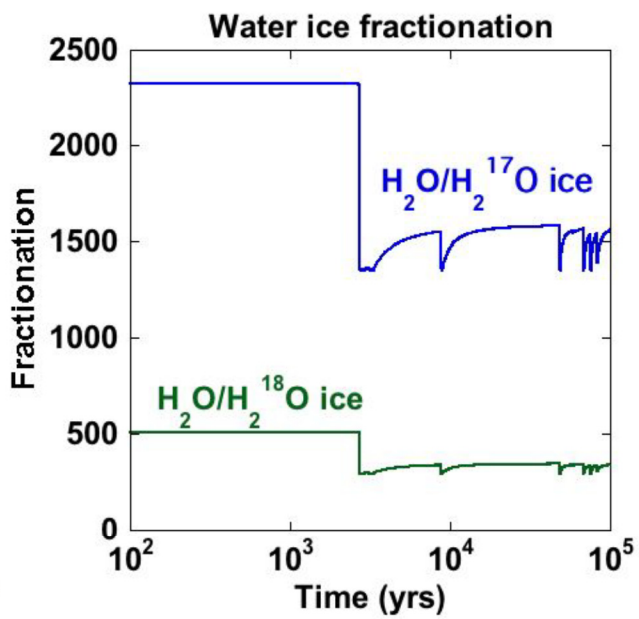

Photodissociation region
(hot gas)
^{17}O, ^{18}O, ^{16}O
dissociation
Dissociation
of C^xO, CO_2
H_2O desorbed
Reform
water and O_2
CO reforms
CO, CO_2
Grain
reactions
form water
High $H_2{}^{16}O/H_2{}^xO$ ice
Low $C^{16}O/C^xO$
Low $C^{16}O_2/C^xO_2$
Low $H_2{}^{16}O/H_2{}^xO$ ice
Low $^{16}O/^{16}O^xO$
Shielded region
(cooler gas)
High $C^{16}O/C^xO$

Mixing effects on CO and water fractionation

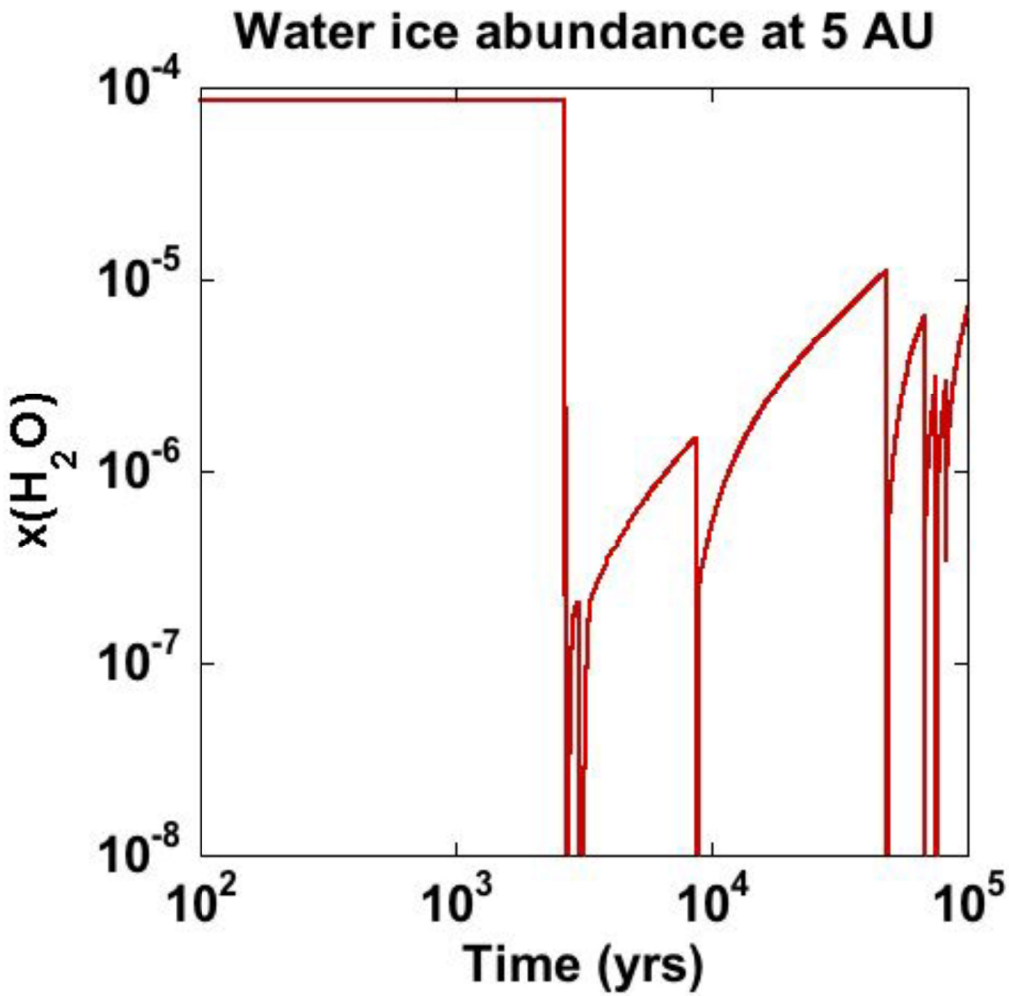








Can mixing lead to a reduction in ice abundances at 5AU?



Summary

- Gas phase deuteration altered by reactions in disk
- Differential photodissociation at surface + mixing important for C and O bearing molecules
  - Explanation for anomalous oxygen isotope ratios in meteorites?
- Vertical mixing (5 AU)
  - Reduces HDO/H_2O ratio in ice by factor of 100

    => better agreement with comet observations
  - Alters oxygen isotope ratios in CO, CO_2 and H_2O
  - May lead to the loss of water ice at 5 AU

    => reduction in mass available for Jupiter formation