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Thermal and Chemical Models of Protoplanetary Disks

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Protoplanetary Disks & Planet Formation

What is the role of thermo-chemical disk models?

- thermo-chemical models help to understand processing and the history of the early Solar System
- observations in conjunction with protoplanetary disk models can be used to trace the location of the gas and its physical properties (density, temperature)
- thermo-chemical disk models put constraints on gas evolution in protoplanetary disks and thus planet formation models (core accretion vs gravitational instabilities)

Outline

- Astrochemistry and protoplanetary disk models
    I. UV irradiation
    II. X-rays
    III. Dust evolution
    IV. Cold gas chemistry
    V. Ices
    VI. Mixing
- Astrochemistry and thermal models
    I. Gas energy balance
    II. Disk structure
    III. Gas dispersal

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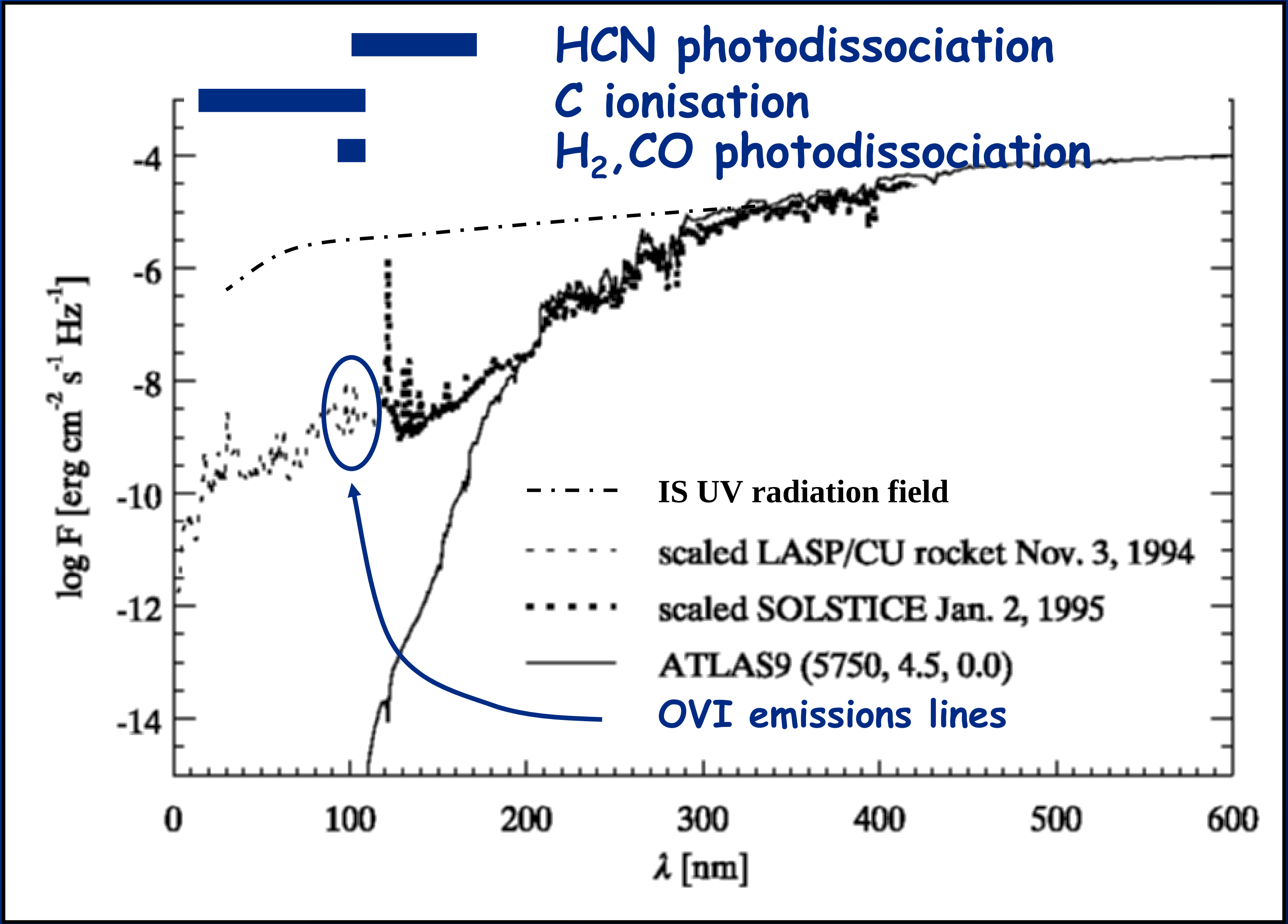
see Alexander talk

UV irradiation

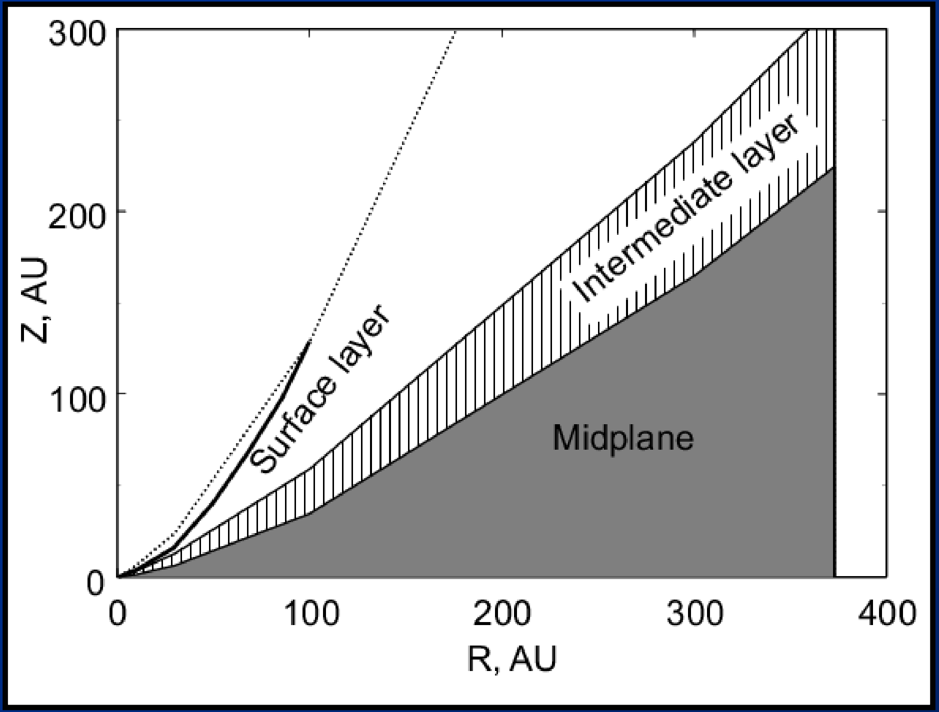


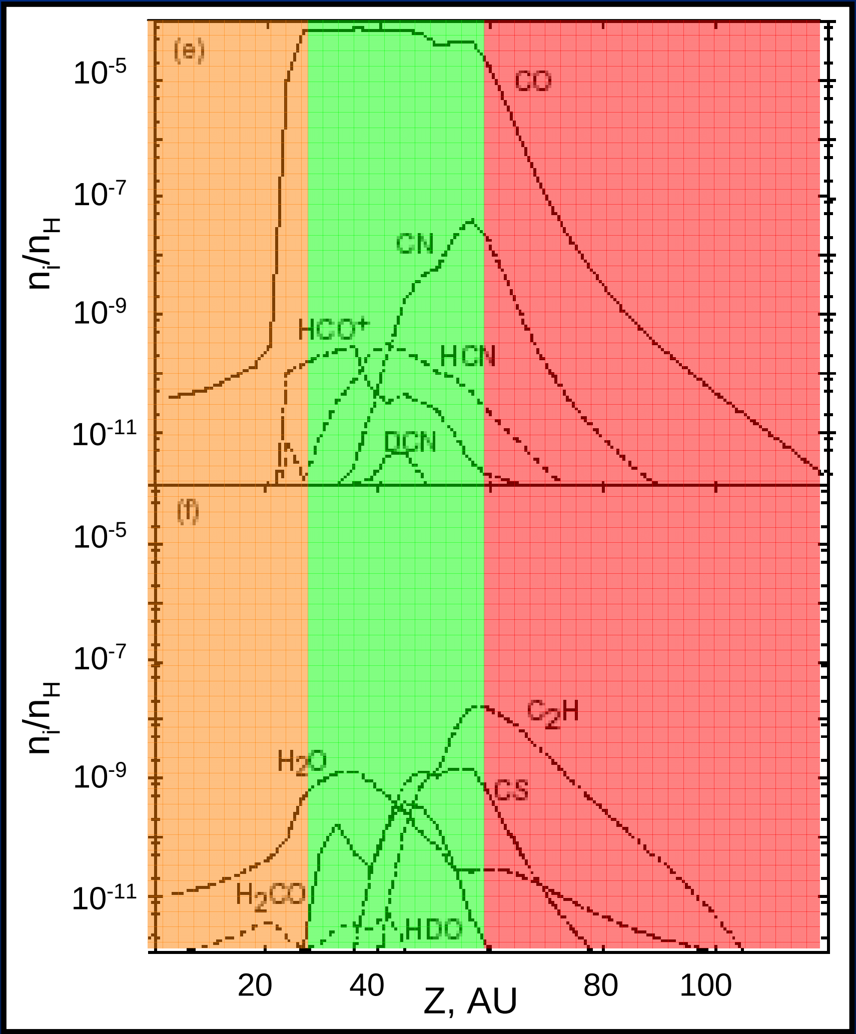
color of stellar radiation field differs from IS UV

[Spaans et al. 1994, Kamp & Sammar 2004]

Gas phase chemistry

surface layer ⮝ photochemistry
intermediate layer ⮝ neutral & ion molecule chemistry
disk midplane ⮝ gas-grain chemistry





[Aikawa & Herbst 1999, Willacy & Langer 2000, van Zadelhoff et al. 2003, Semenov et al. 2004, Kamp & Dullemond 2004, Jonkheid et al. 2004, Nomura & Millar 2005]

Gas phase chemistry

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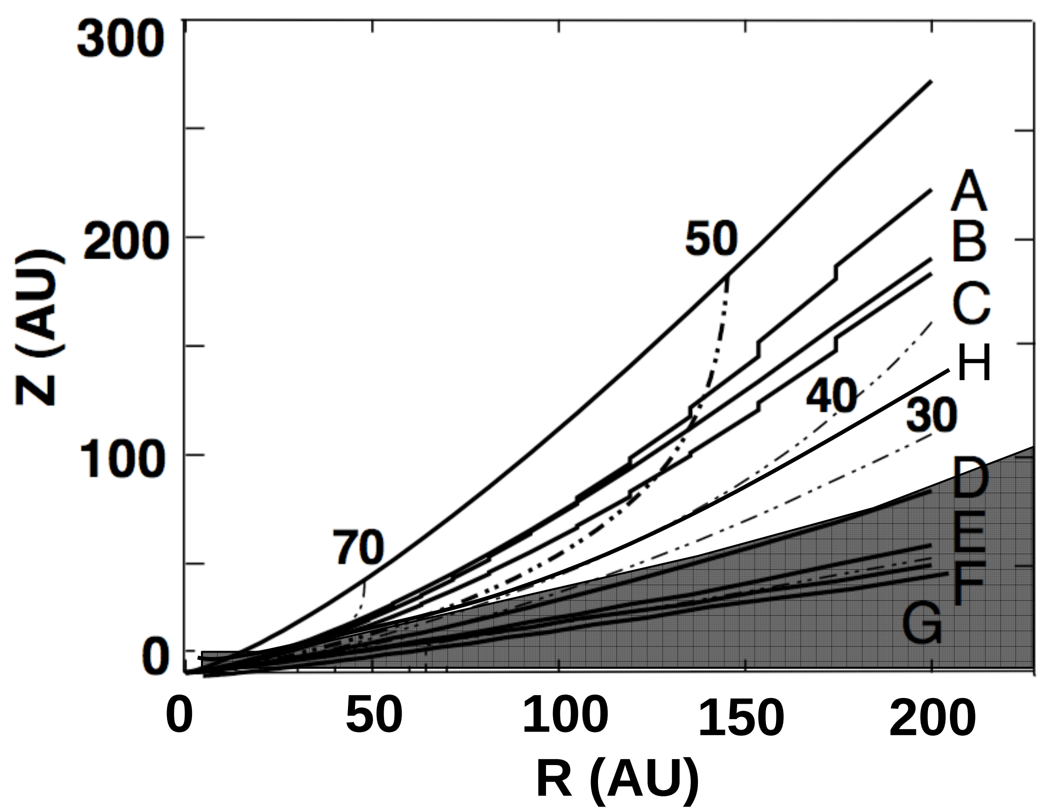
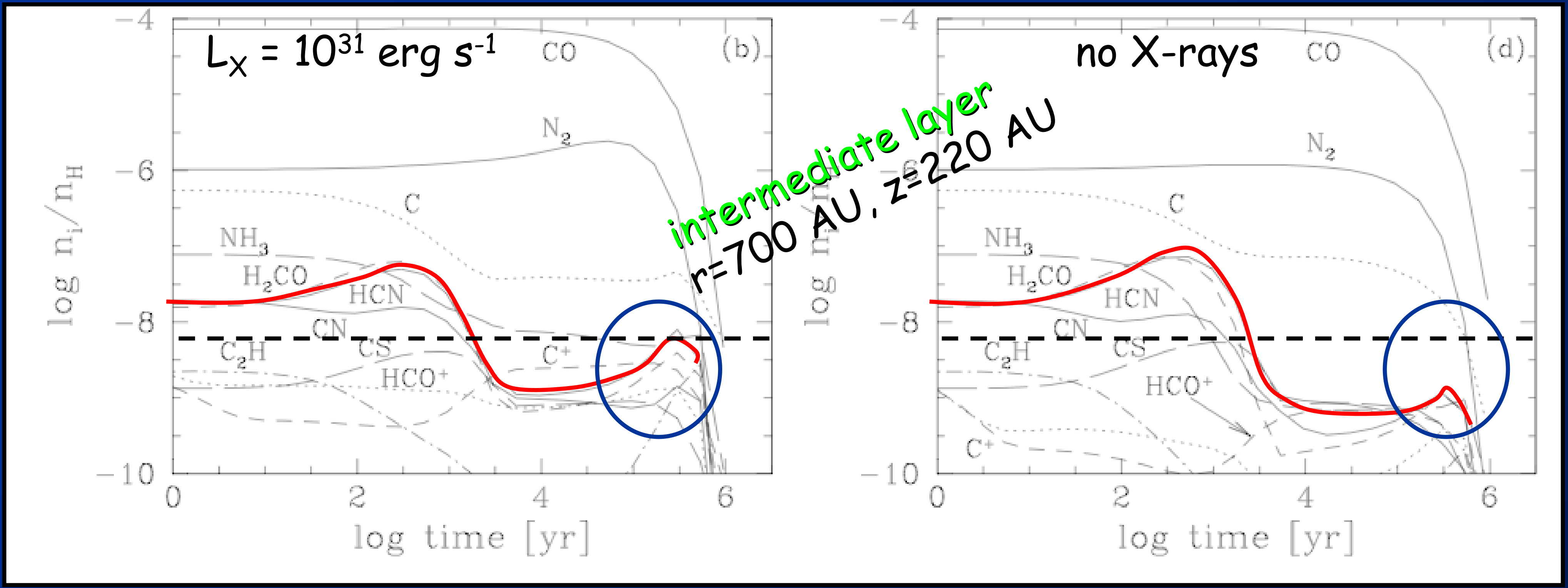


A: ^{12}CO 6-5
B: ^{12}CO 3-2
C: ^{12}CO 2-1
H: HCO^+ 4-5

[van Zadelhoff et al. 2001]

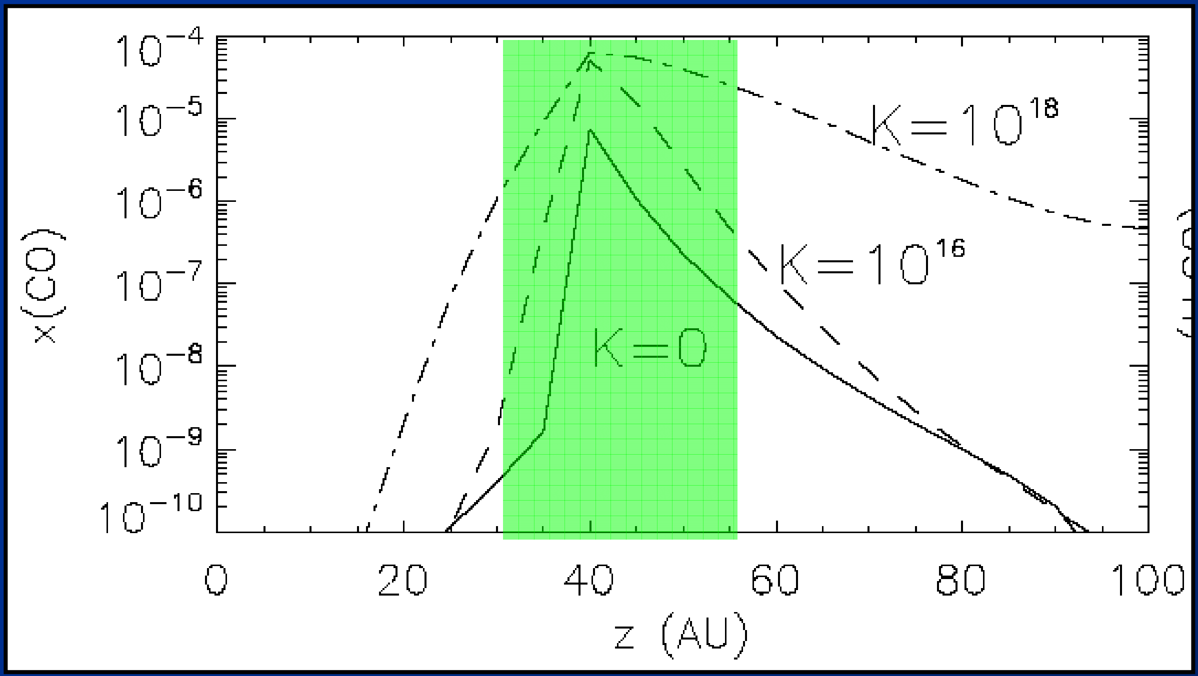
Effects of X-rays

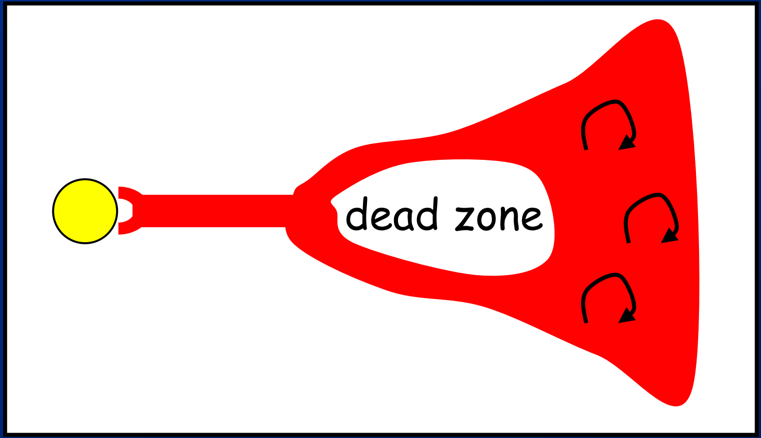


- X-rays enhance the ionization fraction of the disk surface
- many molecules have higher abundances due to efficient ion-molecule chemistry (e.g. HCN)
- L_X/L_{UV} determines the chemical timescales (pure X-ray chemistry takes a factor 100 longer)

[Glassgold et al. 1997, 2004, Aikawa & Herbst 1999, Nomura et al. 2007, Agundez et al 2008]

How does mixing affect the chemistry?





- Mixing has only minor effects on the layered disk structure in the regions > 10 AU
- Mixing affects the vertical column densities of many molecules.
- Mixing can enhance the ionization degree in the dead-zone (r<10 AU)

[Ilgner et al 2004, Semenov et al. 2005, Willacy et al. 2006, Ilgner & Nelson 2006, 2008]

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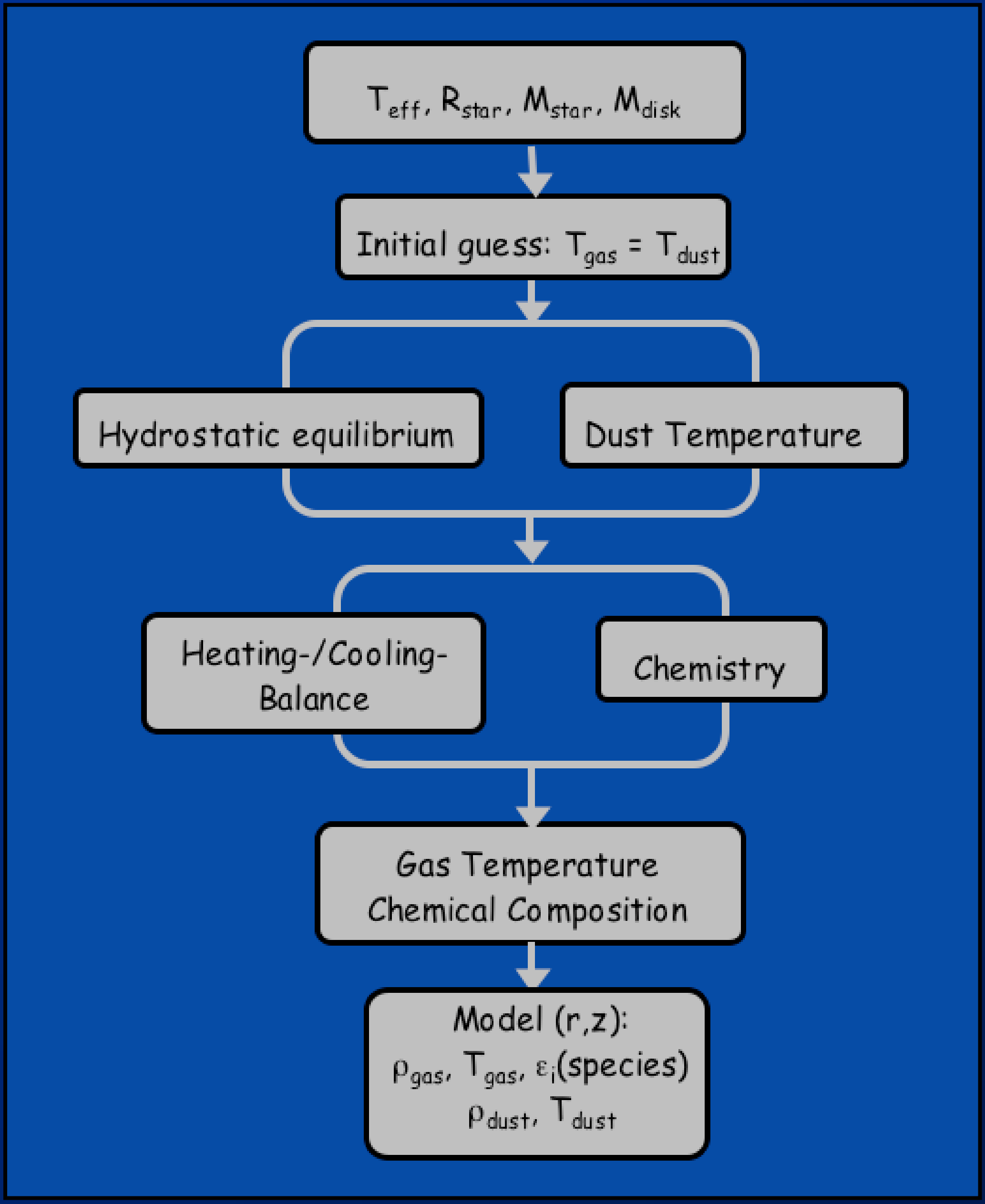
Gas energy balance



Gas energy balance

Heating $\Gamma = \Lambda$ **Cooling**

Heating

Photoelectric heating (grains/PAH)

C ionisation

Cosmic rays

Line pumping by UV/optical/IR background radiation

(X-ray heating)

Collisional de-excitation of H_2^*

H_2 formation/photodissociation

Gas-dust collisions

Cooling

Fine structure line cooling [OI], [CI], [CII]

CO ro-vibrational line cooling

H_2O rotational line cooling

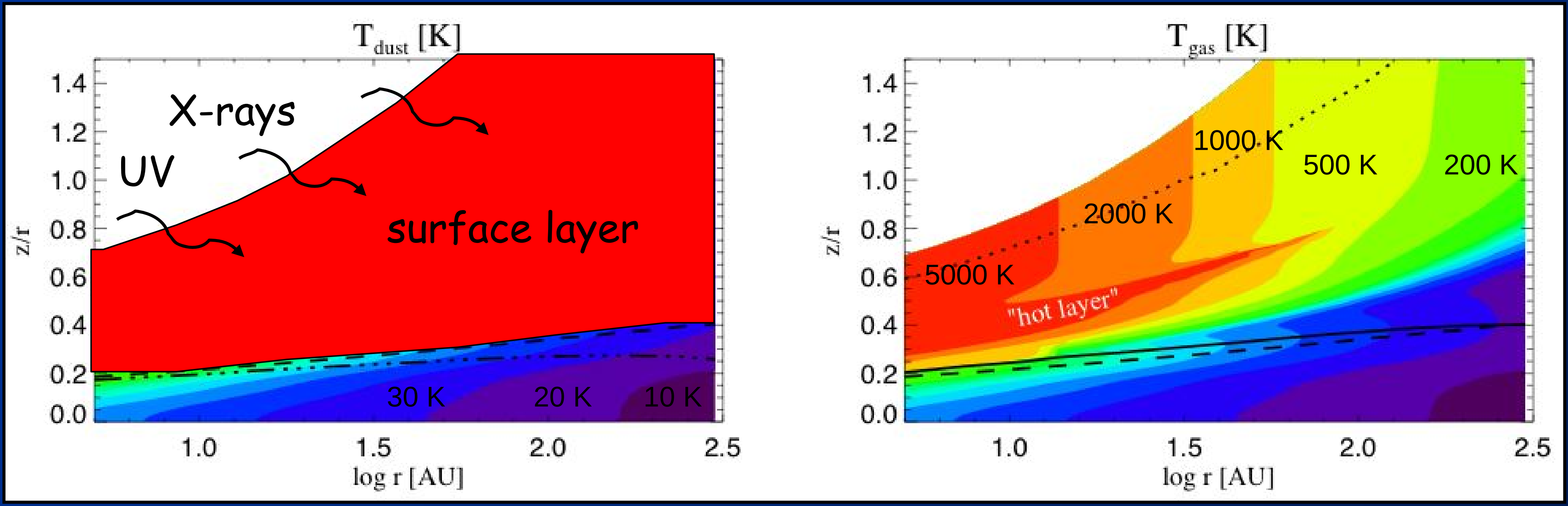
H_2 quadrupole line cooling

Semi-forbidden [SiII], [FeII], [SII]

Lyα, [OI 6300]

Gas-dust collisions

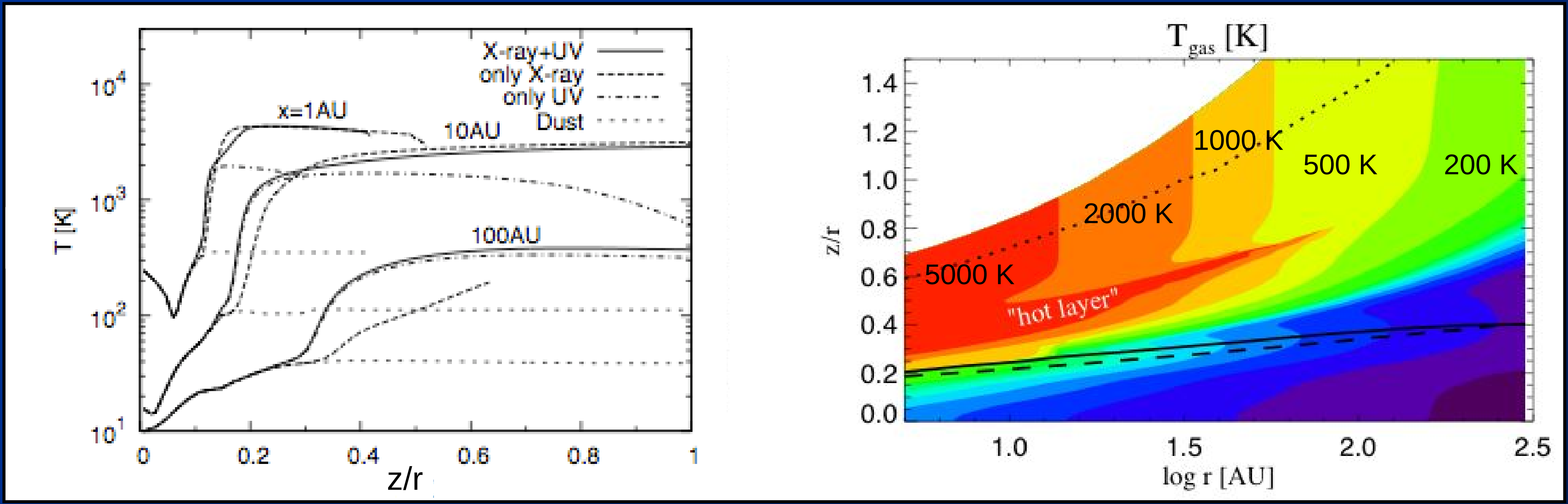
Gas energy balance



- Gas and dust temperature are not coupled in the surface
- X-rays dominate in the inner disk depending on L_X/L_{UV}
- Transition to molecular species occurs before the disk becomes optically thick.

[Kamp & Dullemond 2004, Jonkheid et al. 2004, Nomura et al. 2007]

Gas energy balance



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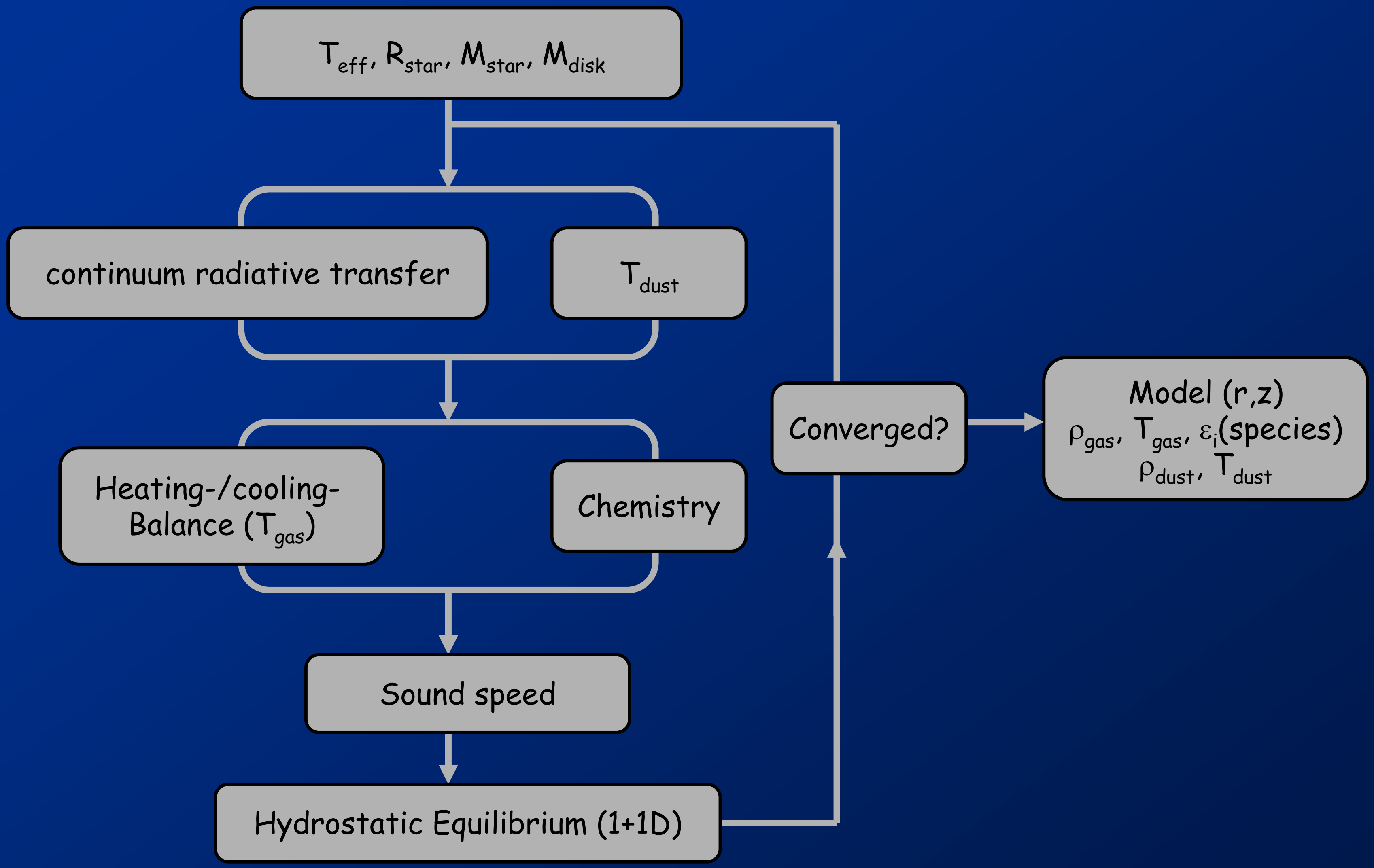
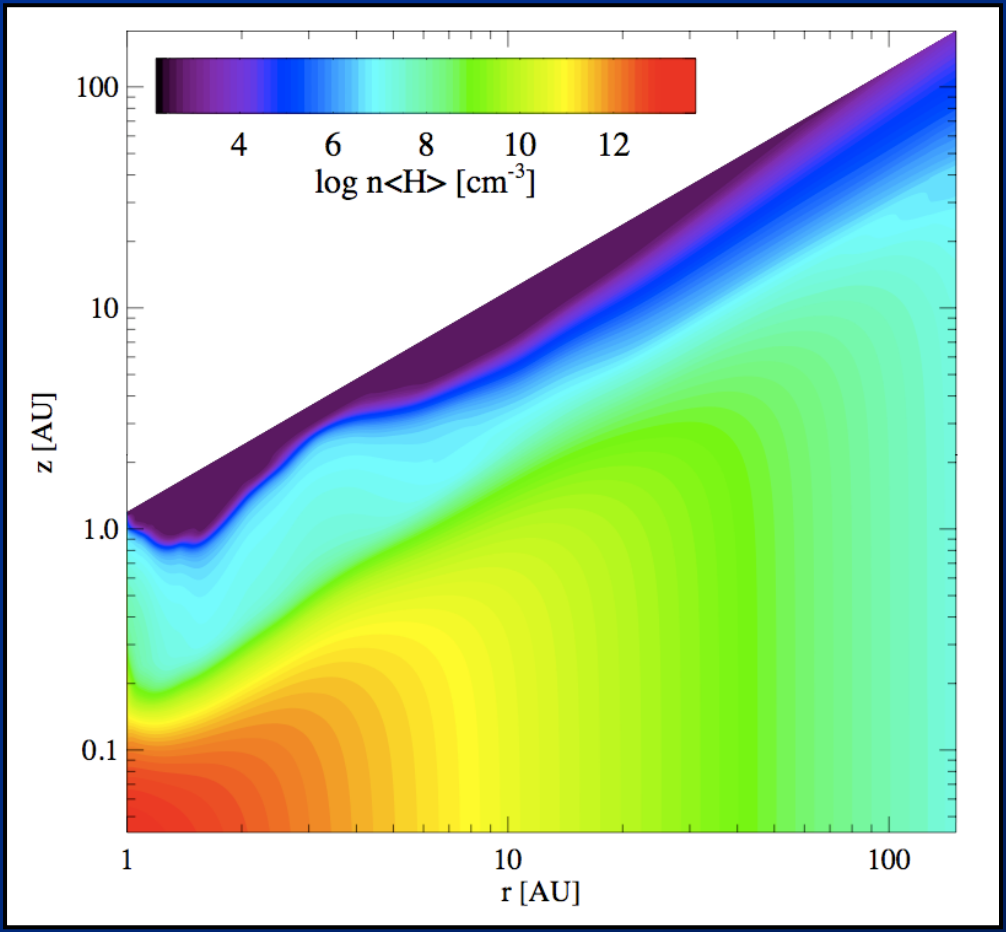
Disk structure



[Gorti & Hollenbach 2004, Nomura & Millar 2005, Woitke, Kamp & Thi in preparation]

Disk structure



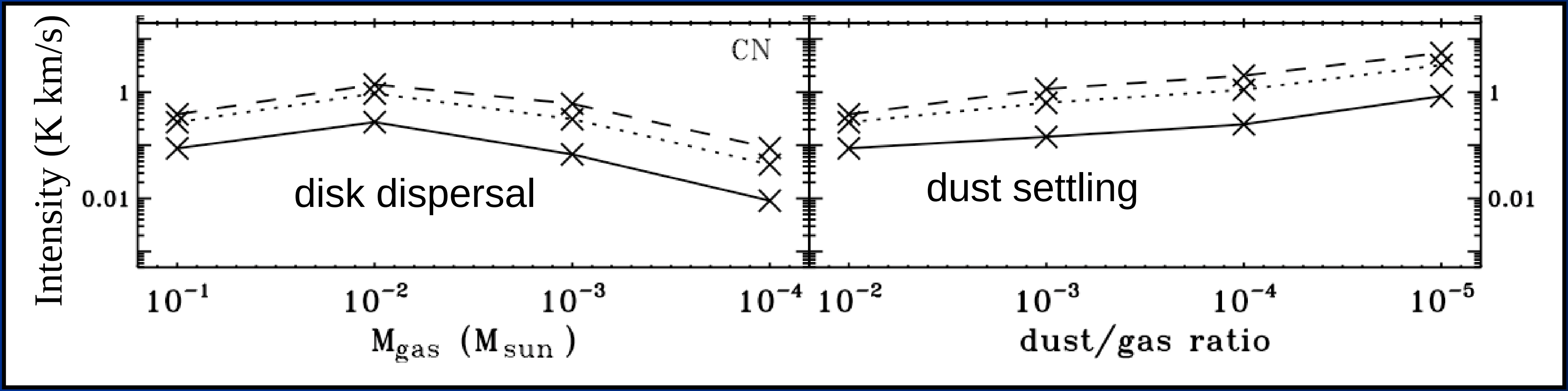
- vertical disk structure is set by T_{gas}
- surface layers are more flaring than in T_{gas}=T_{dust} models

[Woitke, Kamp & Thi in preparation]

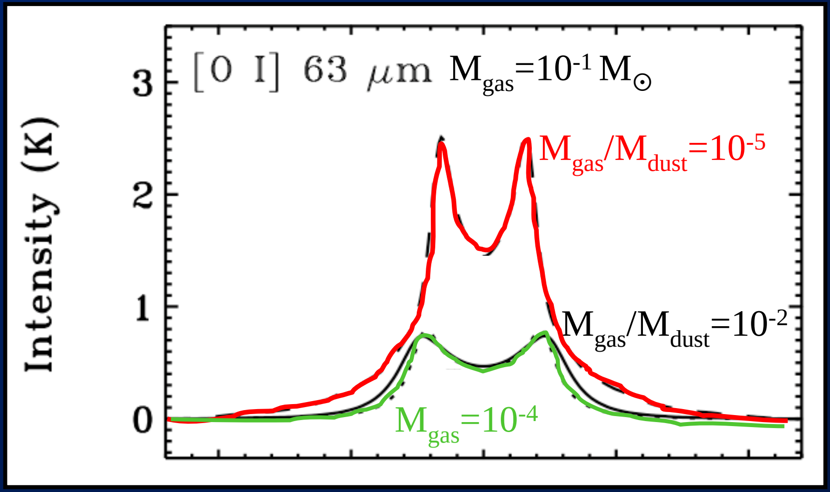
Future work:

- realistic dust evolution (growth and settling) in thermo-chemical modeling
- realistic gas opacities for the disk energy balance (inner disk)
- ice formation and desorption, surface chemistry (outer disk)
- radial and vertical mixing (if indicated by observations)
- Observations, observations, observations to constrain the models !

Effect of dust evolution

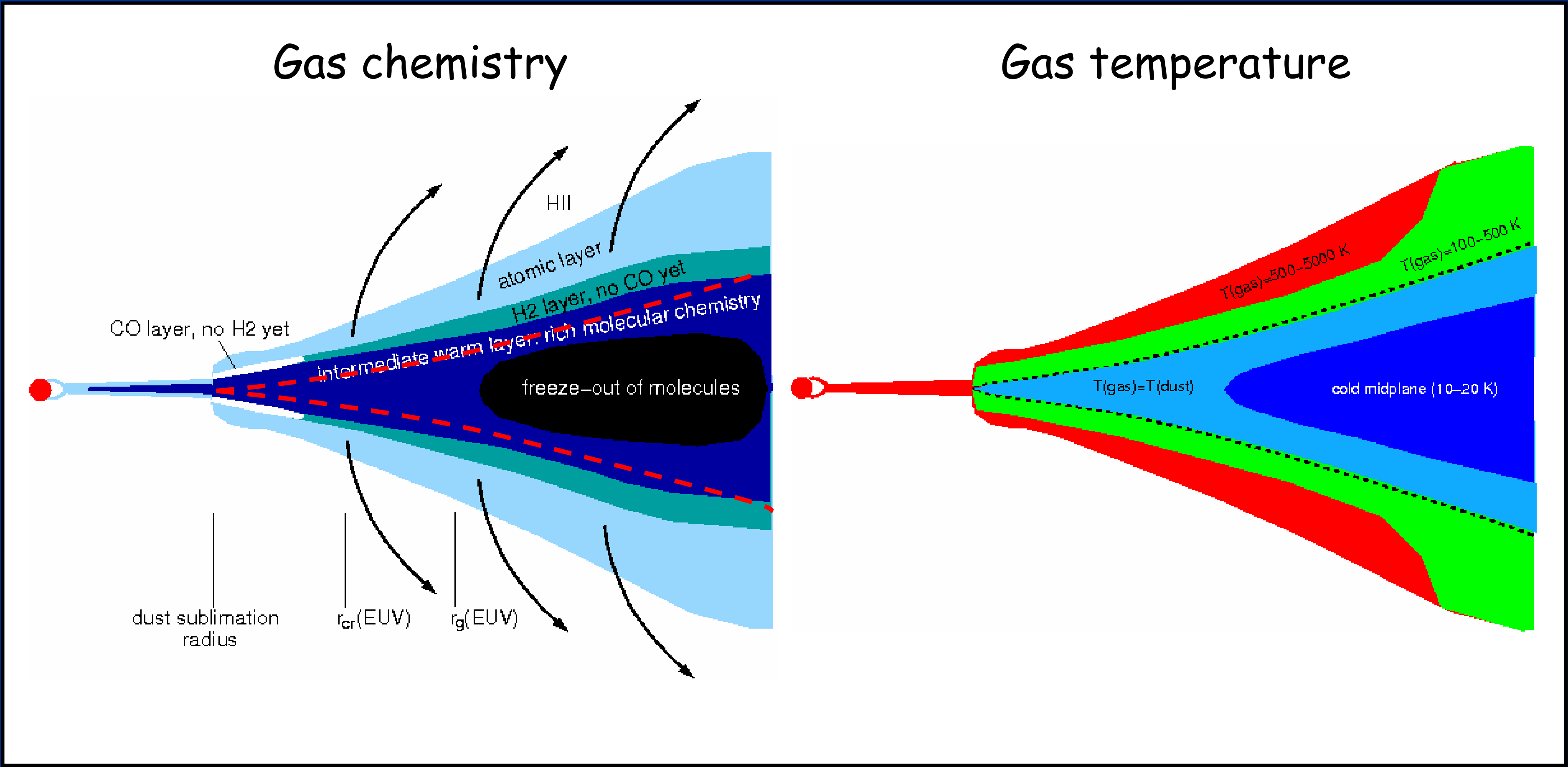


- Dust settling lowers the gas temperature in the surface (less photoelectric heating)
- Grain growth lowers the gas temperature in the surface but warms up the intermediate layers



[Aikawa & Nomura 2006, Jonkheid et al. 2007]

Summary



layered chemical and temperature structure:

hot atomic surface
warm intermediate layer
cold disk midplane

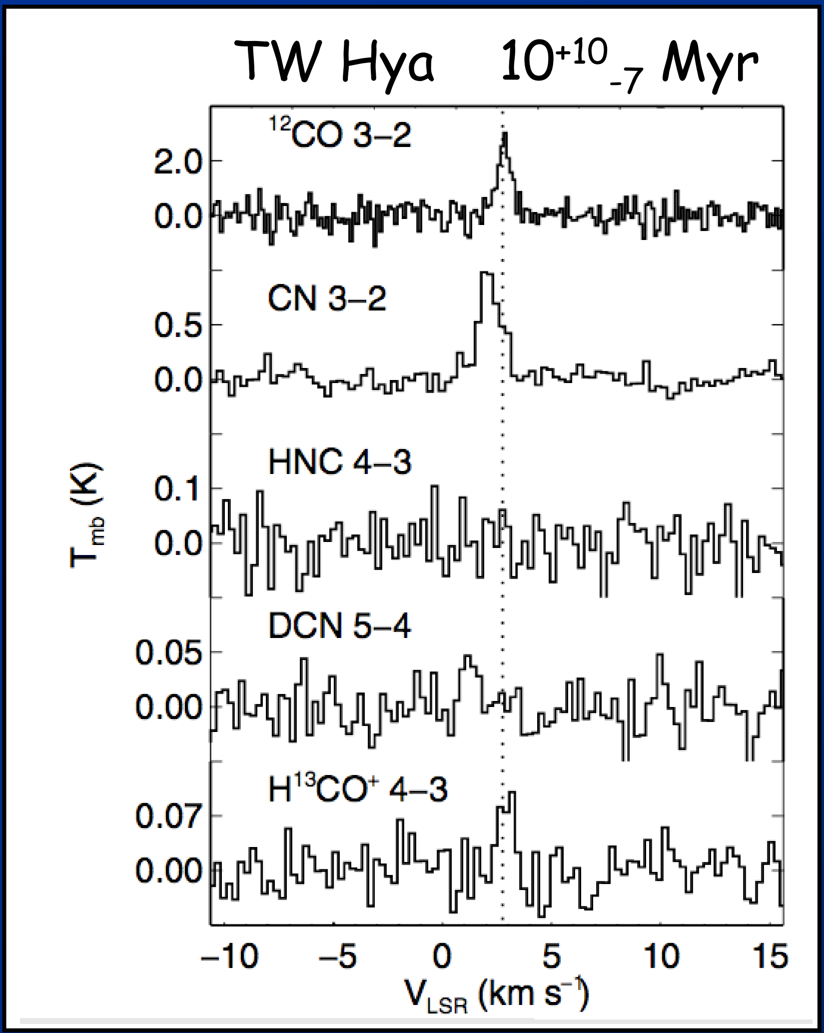
[Dullemond, Hollenbach, Kamp, D'Alessio 2007]


Thanks !
Photo: ESA

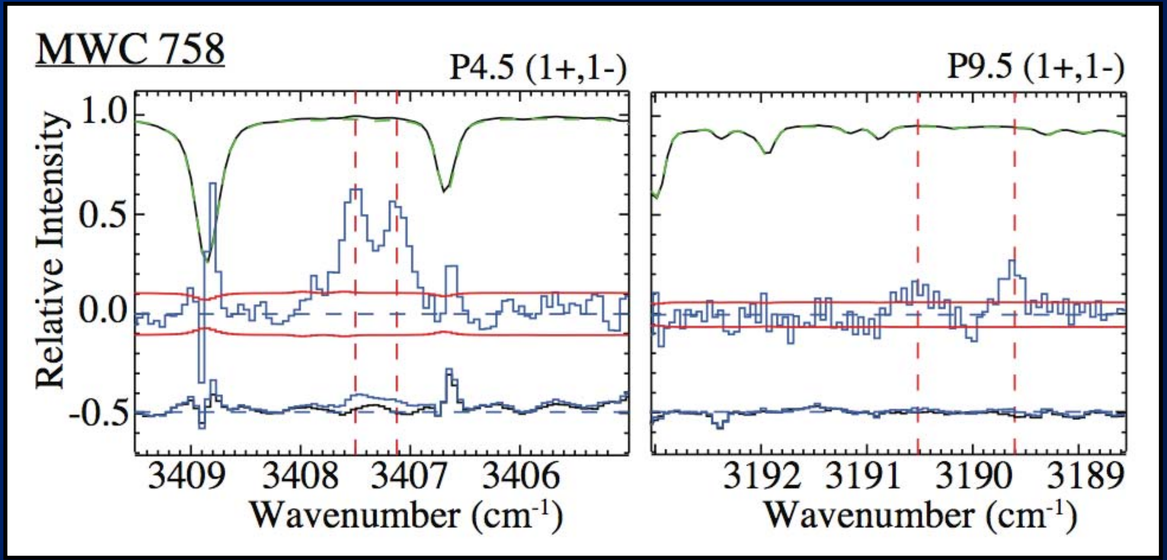
Conclusions:

- Chemistry of outer protoplanetary disks driven by irradiation photochemistry (surface), X-ray chemistry, CR ionization
- Chemistry of inner protoplanetary disks driven also by dynamics accretion flows, turbulent mixing and diffusion
- Chemical signatures can get reset in the disk stage (alternative: pristine from molecular clouds/dark cold cores)
- SOFIA, Herschel and ALMA will facilitate the detection of gas/ice in transition phase disks and spatially resolve them
  ➲ comparison with Solar System chemistry
- VLT/VISIR, ISAAC, CRIRES probe the inner disk material
  ➲ gas dispersal and planet formation

Gas phase chemistry



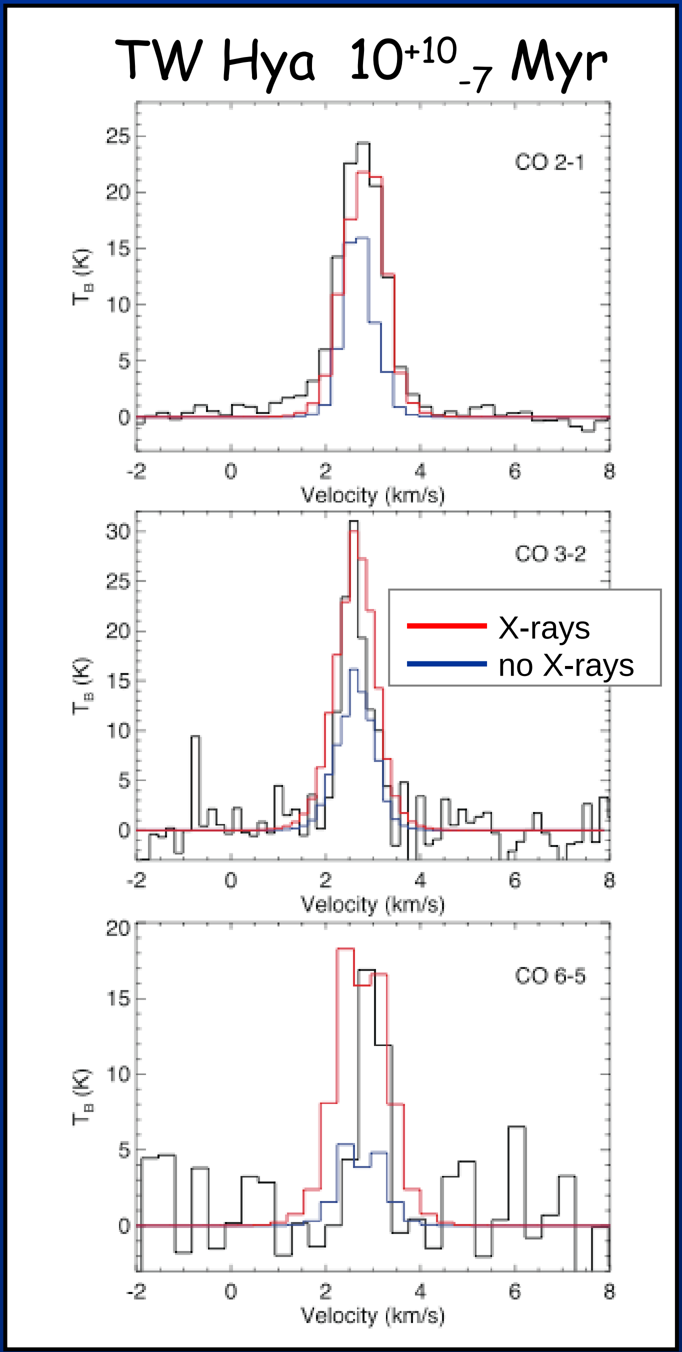
- CN and HCO+ indicate UV irradiation
- origin in warm intermediate disk layer (ion-molecule chemistry)
- OH from inner disk (1-2 AU, T~750 K) indicates UV/NIR irradiation



[Thi et al. 2004]

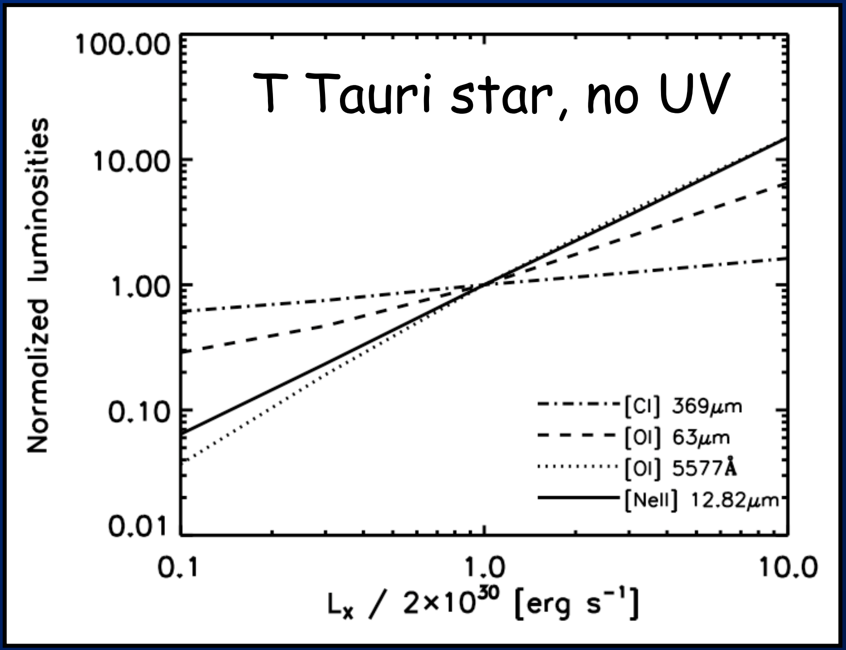
[Manddell et al. 2008]

Effects of X-rays



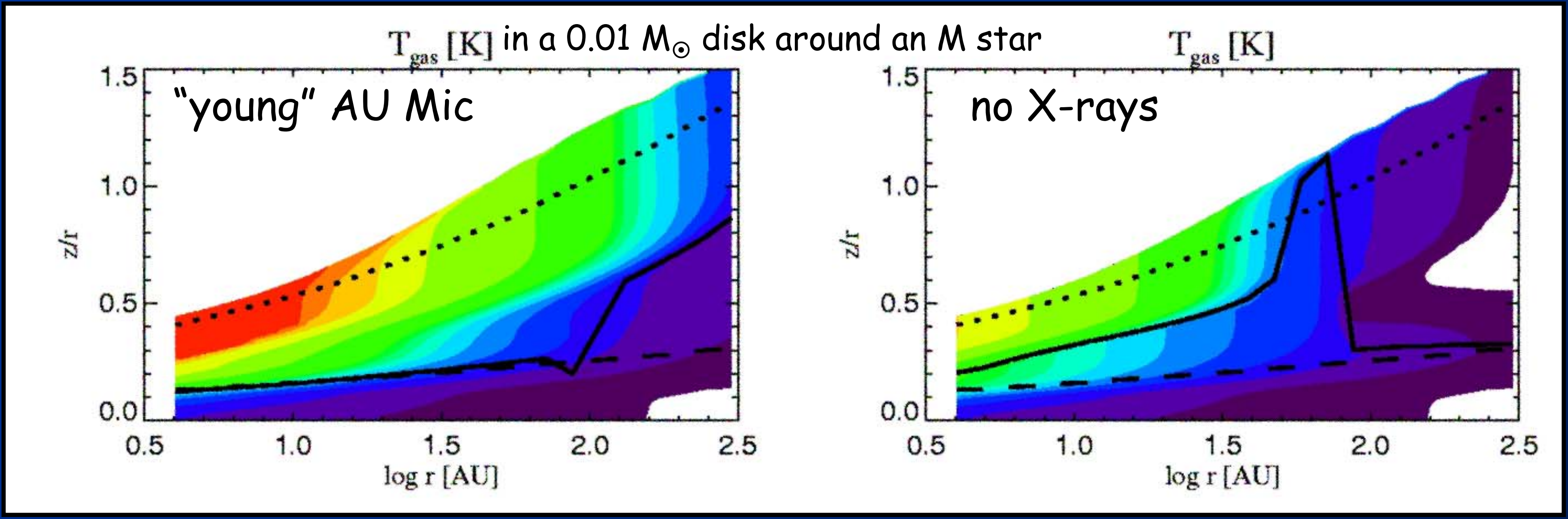
- X-rays affect molecular line emission, especially line ratios (e.g. CO, H_2)

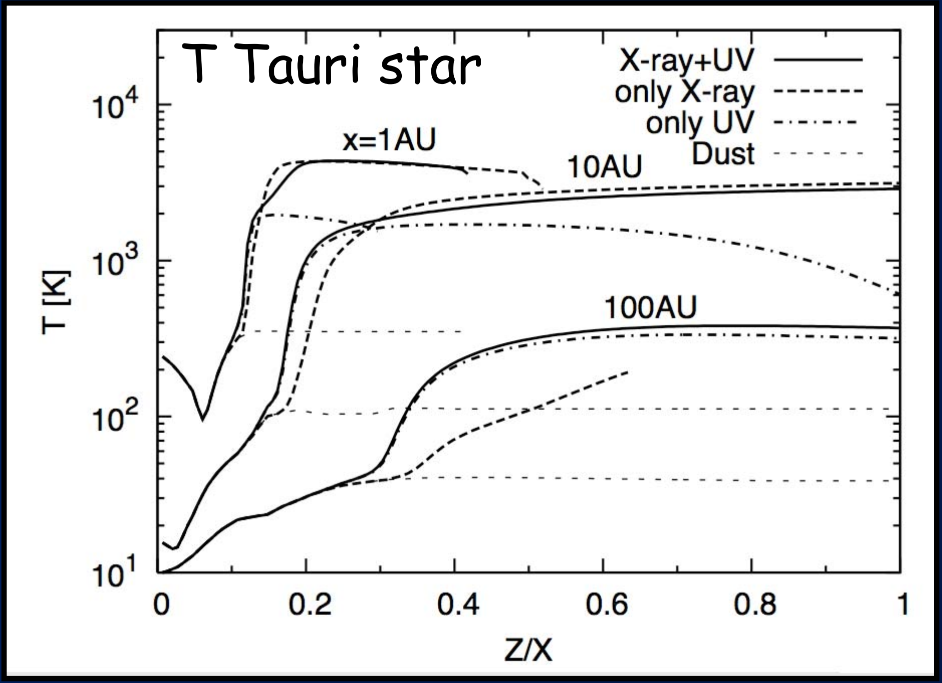
  and also fine structure lines originating from the inner disk (r<25 AU) such as [NeII], [OI]



[Qi et al. 2006, Nomura et al. 2007, Meijerink et al. 2008]

Effects of X-rays





- X-rays can efficiently heat the gas in the disk surface

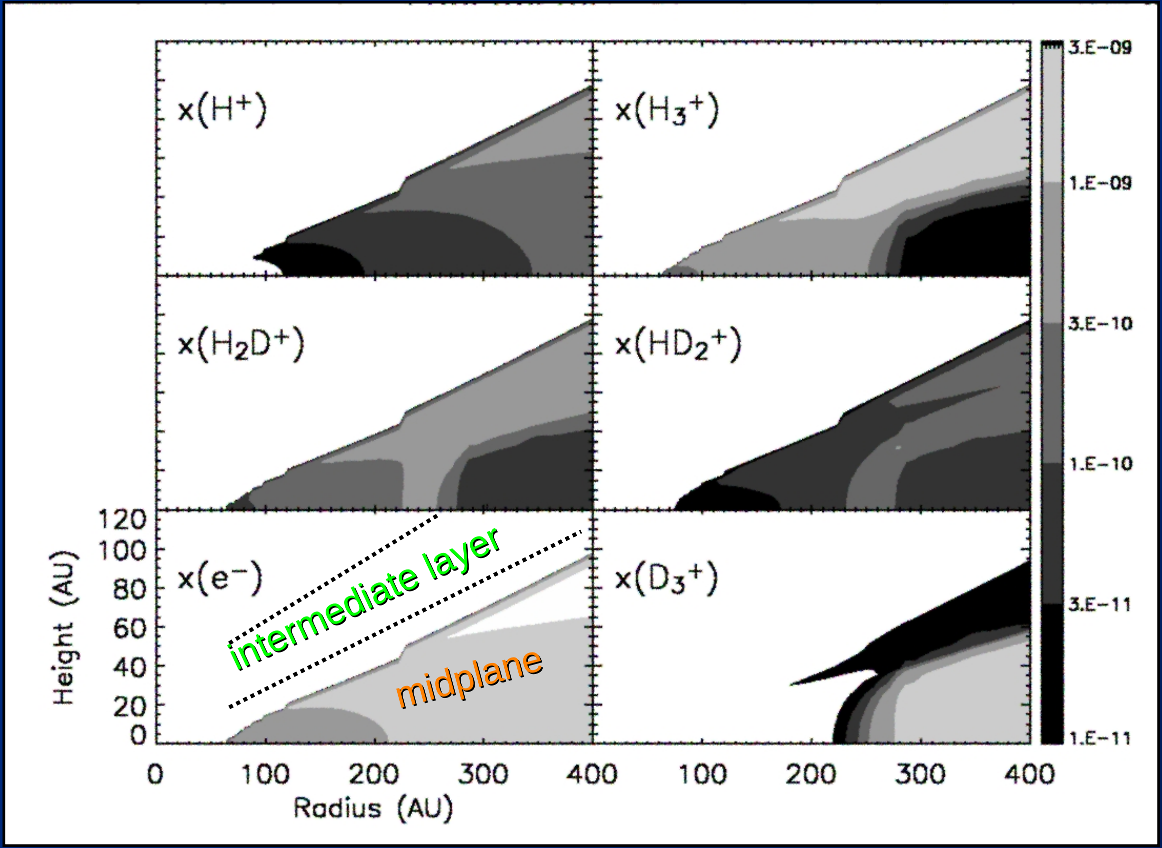
[Glassgold et al. 2004 , Kamp et al. 2005, Nomura et al. 2007]

Deuterium Chemistry

H_3^+ is formed by cosmic rays (UV and X-rays do not penetrate deep)

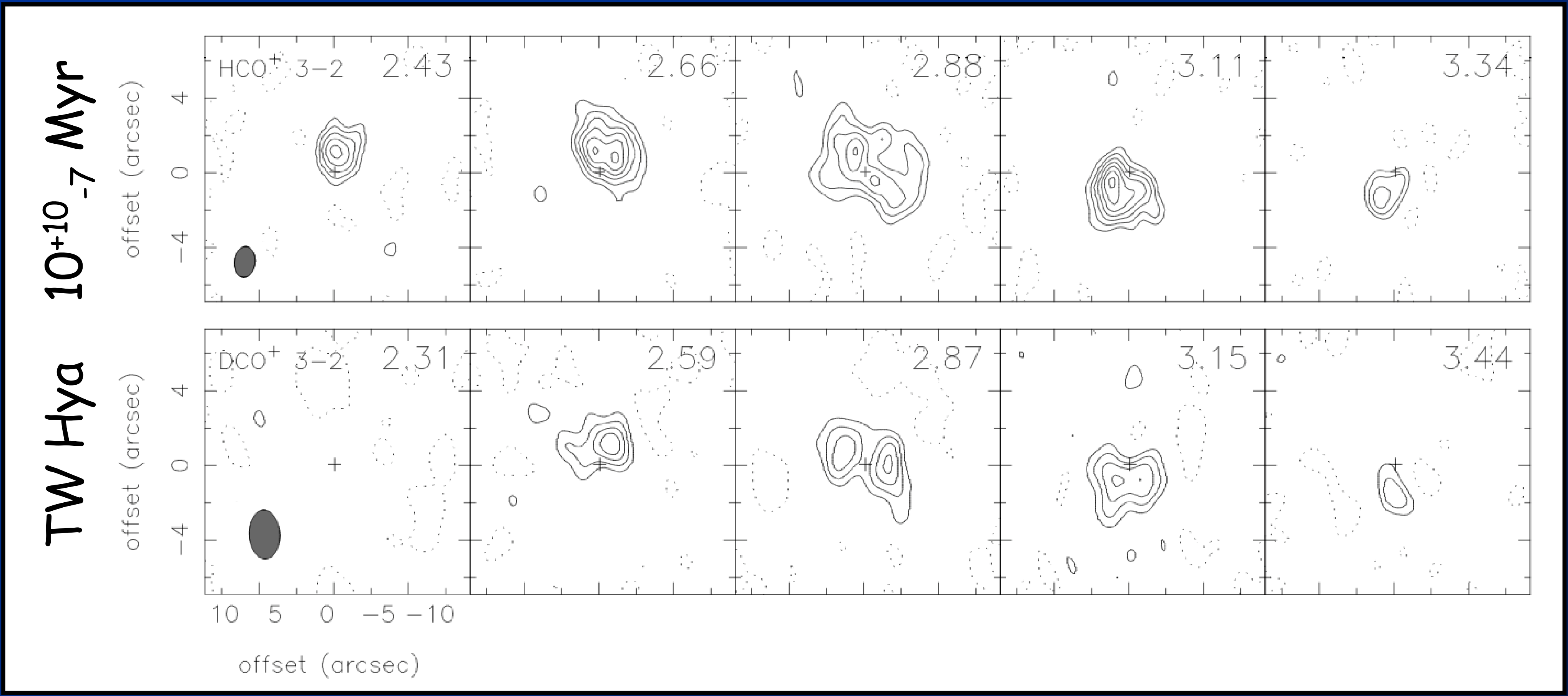
$$H_3^+ + HD \rightarrow H_2D^+ + H_2$$
$$H_2D^+ + HD \rightarrow HD_2^+ + H_2$$
$$HD_2^+ + HD \rightarrow D_3^+ + H_2$$

[Aikawa & Herbst 1999, 2001, Ceccarelli & Dominik 2005, Willacy 2007]



- D/H in molecules is higher than the elemental D/H ratio in the ISM
- Destruction via grain surface recombination and reactions with CO, N_2
- Deuteration increases with distance from the star

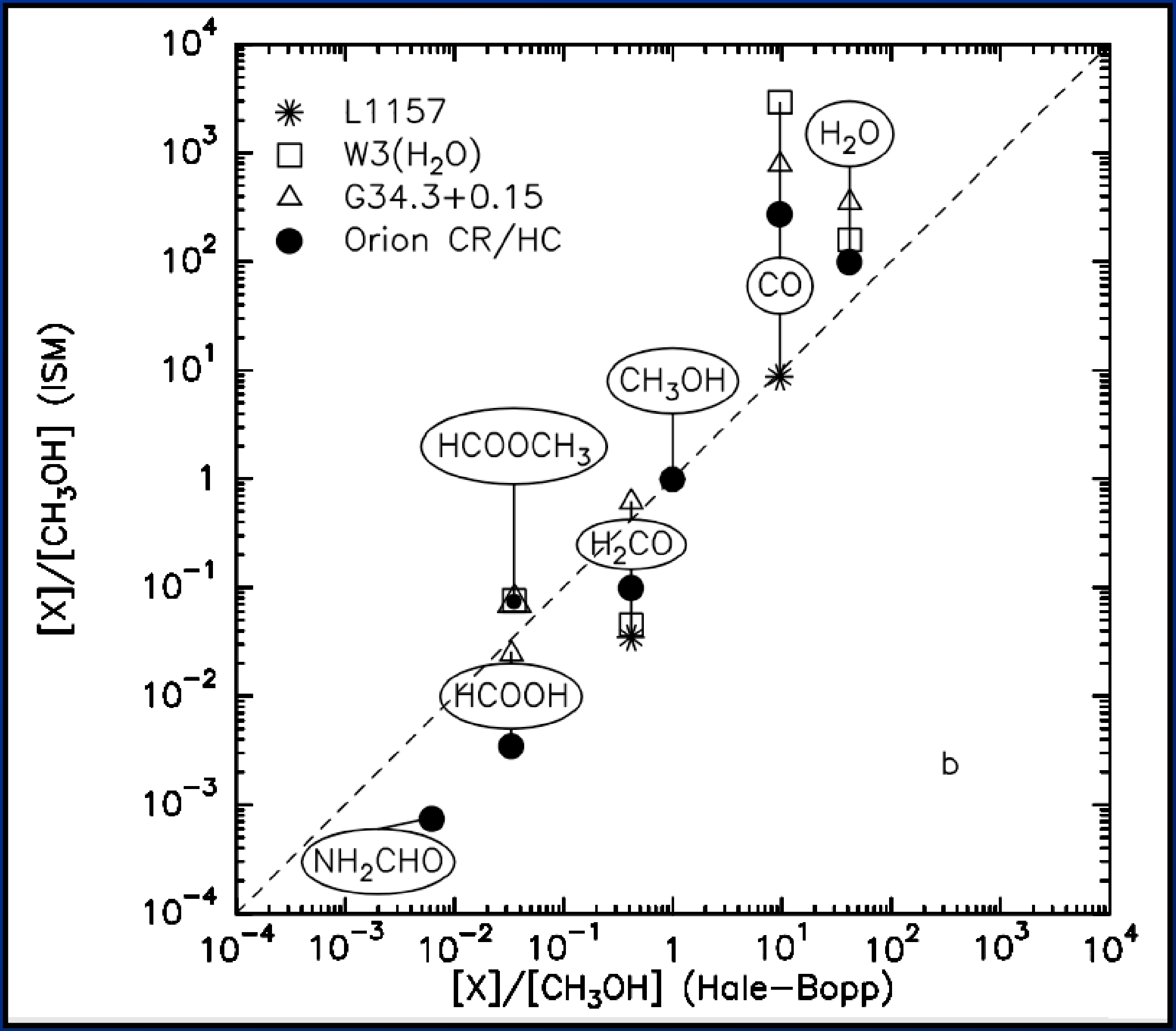
Deuterium Chemistry



[van Dishoeck 2003, Thi et al. 2004, Qi et al. 2008]

- D/H ratio ~ 0.017-0.035
- higher than ISM, but similar to dark cold cores and comets
- D/H ratio reset in protoplanetary disks

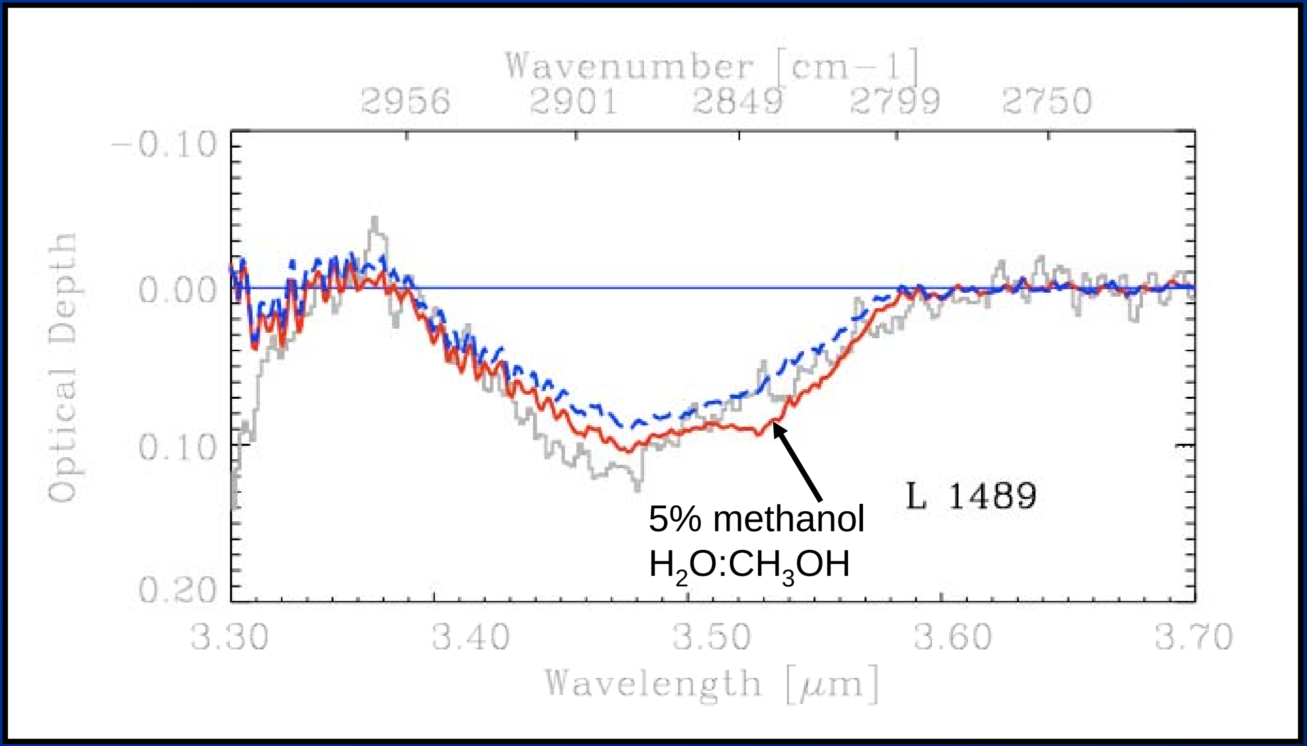
Cold Gas-Grain Chemistry



- Striking similarity between comets and ISM
- Comets form in the outer protoplanetary disk (r > 30 AU)
- Similar cold chemistry as in ISM including deuterium fractionation
- Limit to additional processing such as shocks and strong mixing

[Aikawa & Herbst 1999, Bockelee-Morvan et al. 2000, Rodgers & Charnley 2002]

Ices in Disks



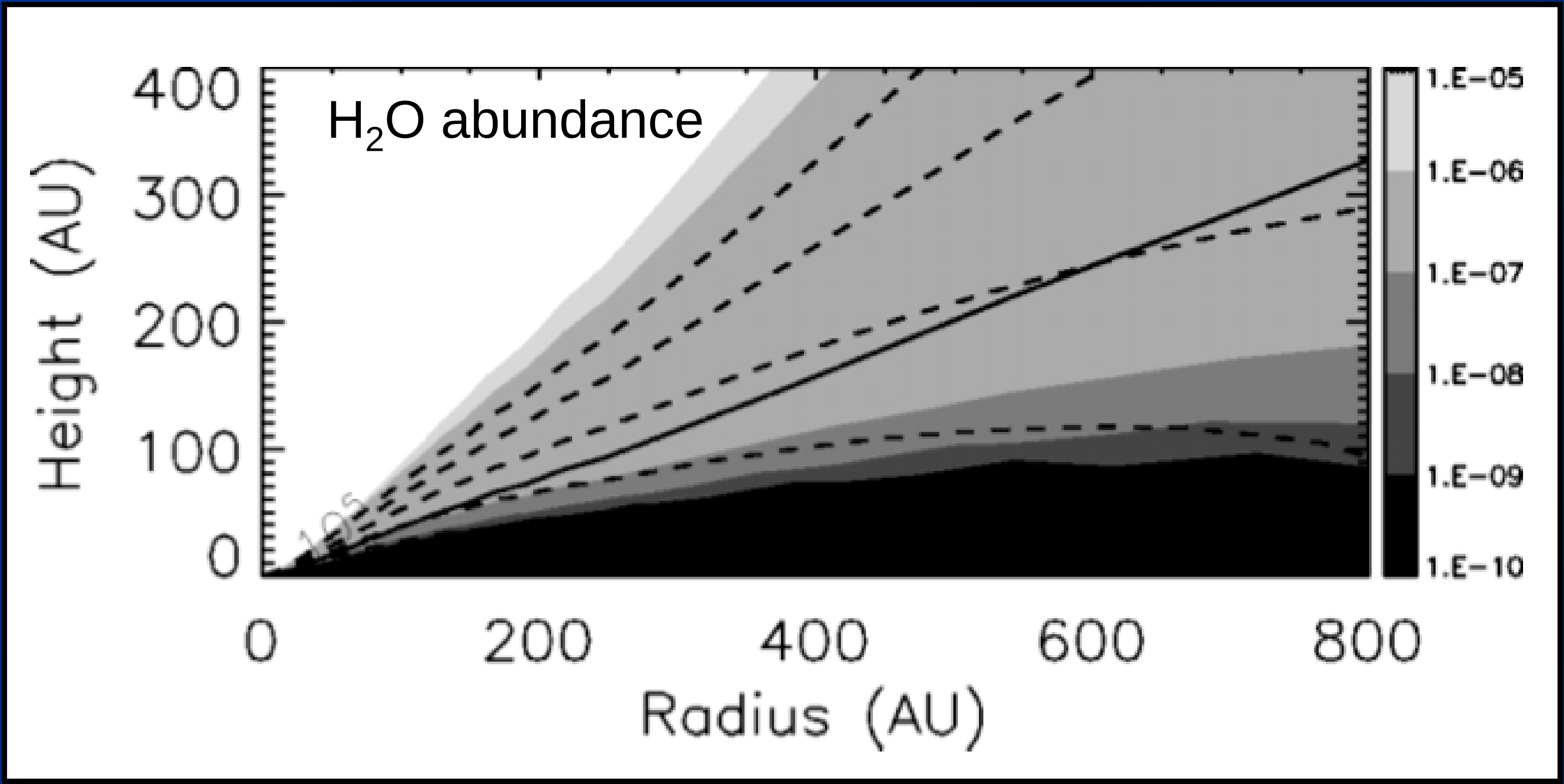
edge-on disk (class I)

upper limit of 5% to the methanol content in the ice

- H_2O ice abundance in disks ~ 10^{-4} (relative to H_2)
- CO_2 and CO ice (CO only mixed with H_2O ice)

[Boogert et al. 2002, Thi et al. 2002, Watson et al. 2004, Pontoppidan et al. 2005]

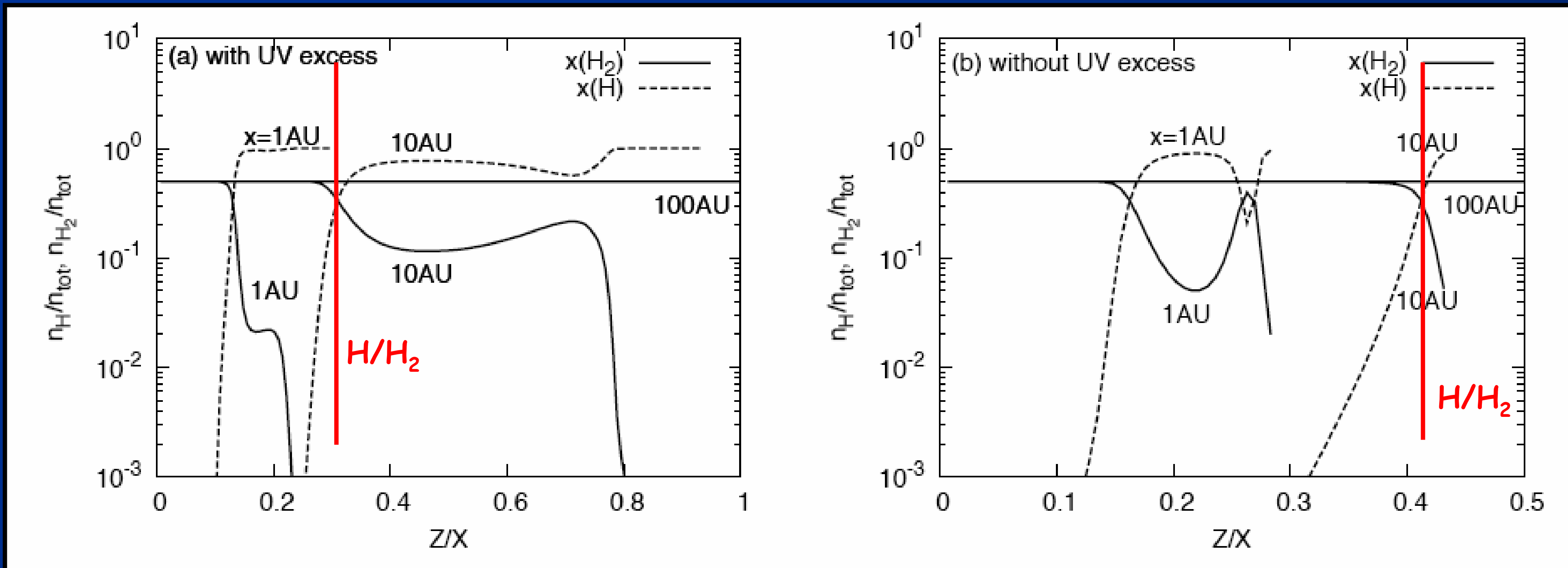
Ices in Disks



- photodesorption of ices in the irradiated disk surfaces
- non-thermal desorption by cosmic ray heating
- H_2O gas column densities 1-2 10^{15} cm^{-2}

[Dominik et al. 2005, Willacy 2007]

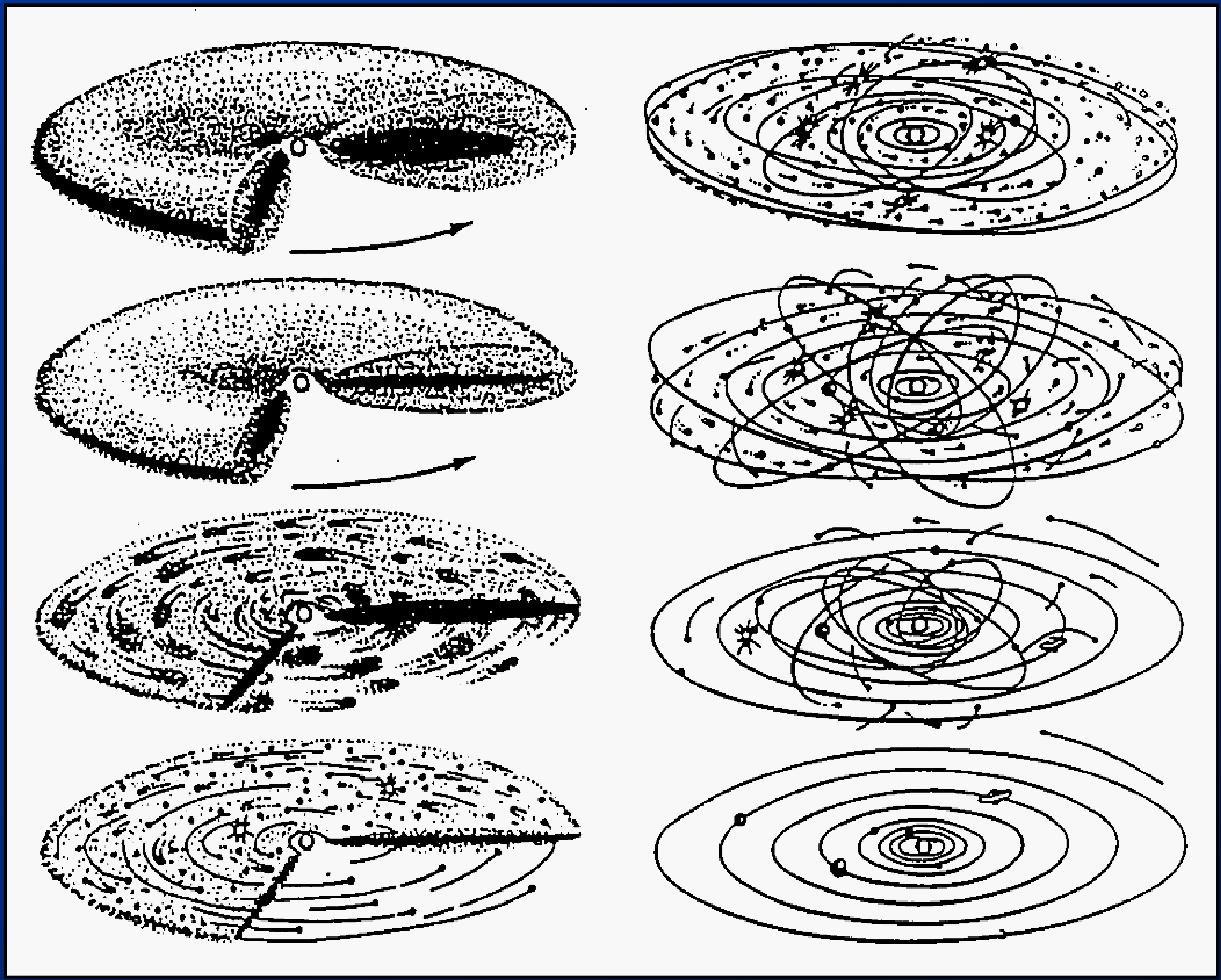
Gas energy balance



- Chemical destruction of H_2: $H_2 + O \rightarrow H + OH$
- C/CO transition at lower/same optical depth as H/H_2 transition
- Higher UV fluxes lead to lower molecule abundances in the disk atmosphere

[Kamp & Dullemond 2004, Nomura & Millar 2005]

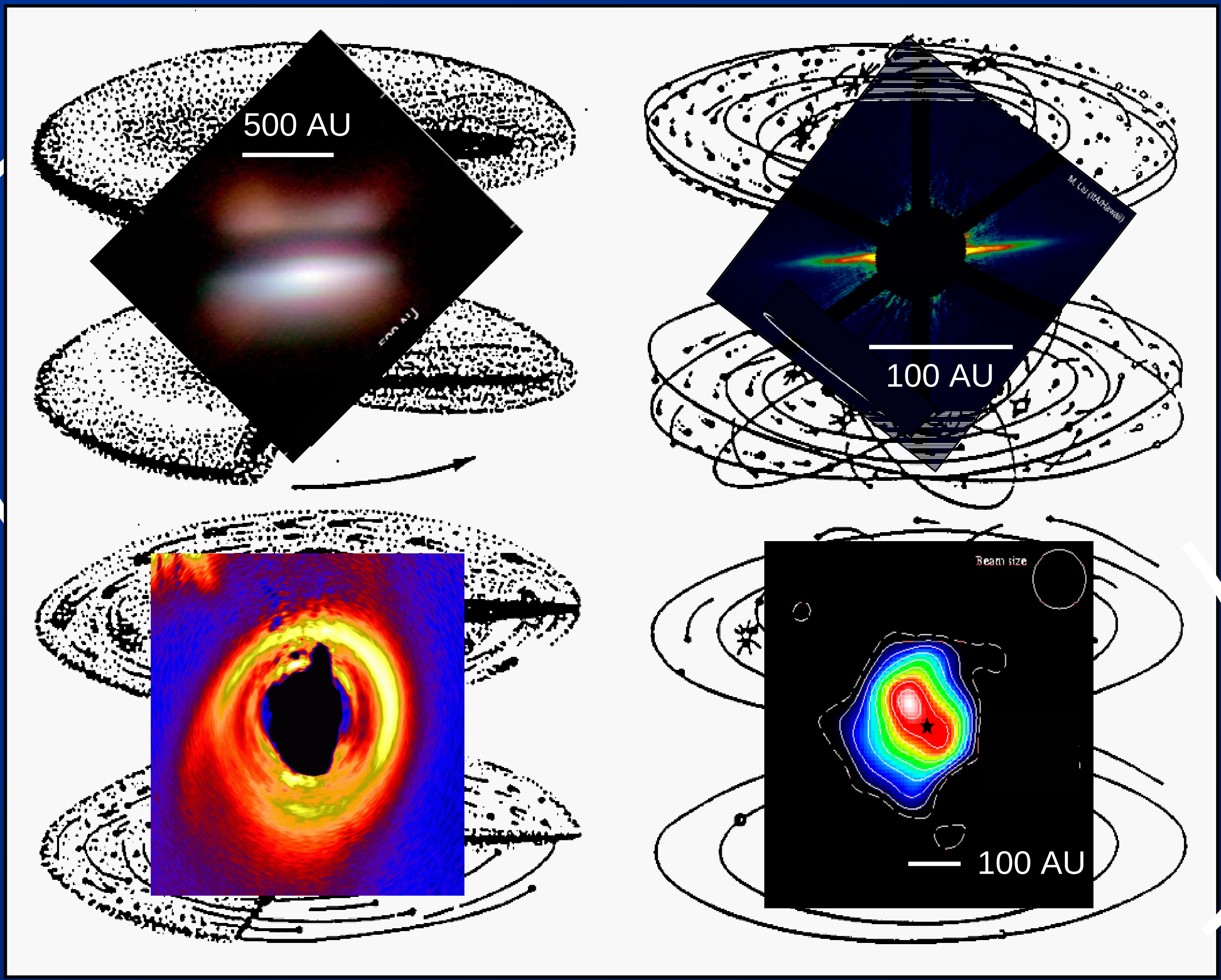
Protoplanetary Disks & Planet Formation



Protoplanetary Disks & Planet Formation

gas
+
dust

gas (?)
+
dust



gas (?)
+
dust

debris
disk
/
zodiacal
dust

Protoplanetary Disks & Planet Formation

gas
+
dust

gas (?)
+
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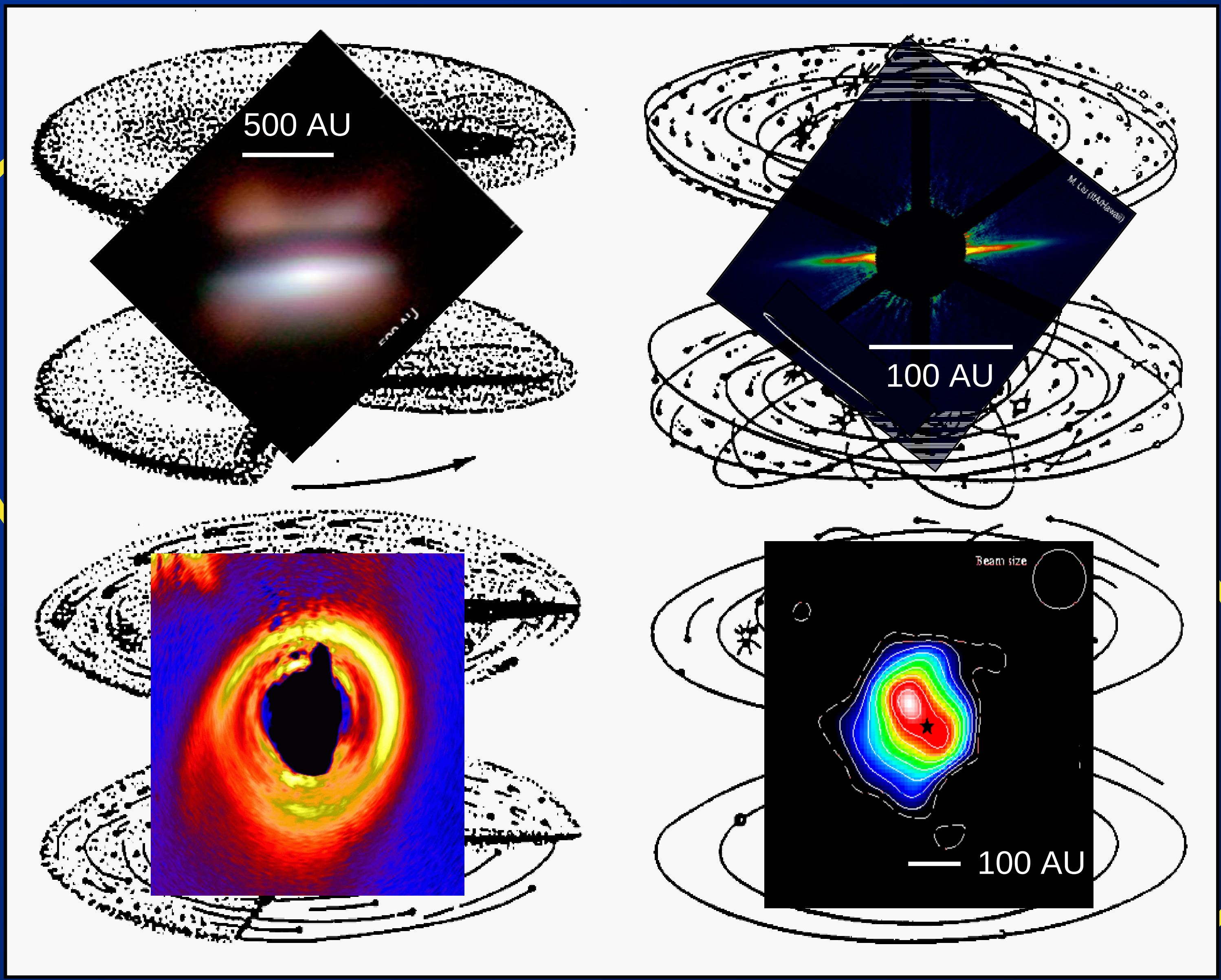

gas (?)
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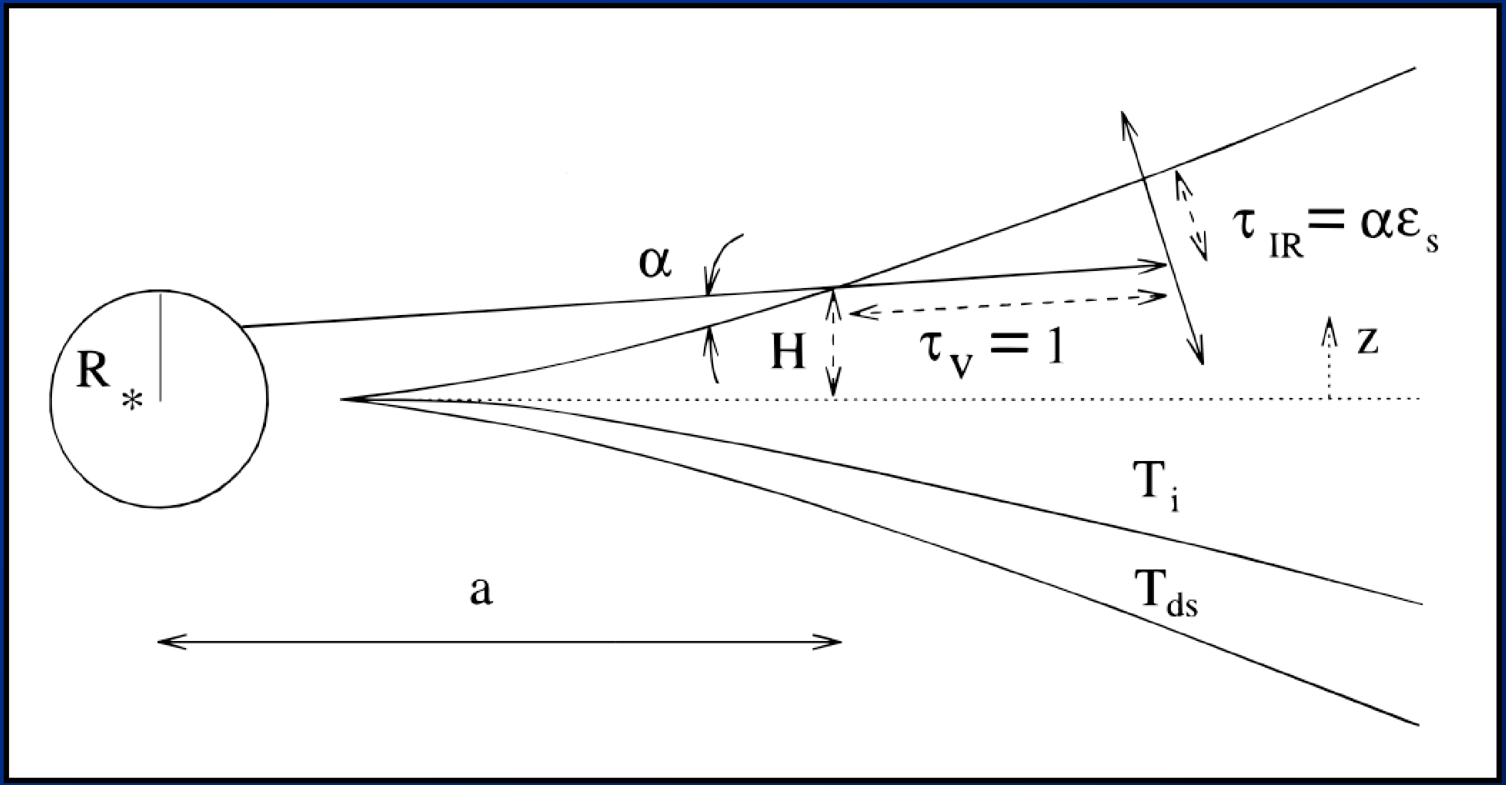
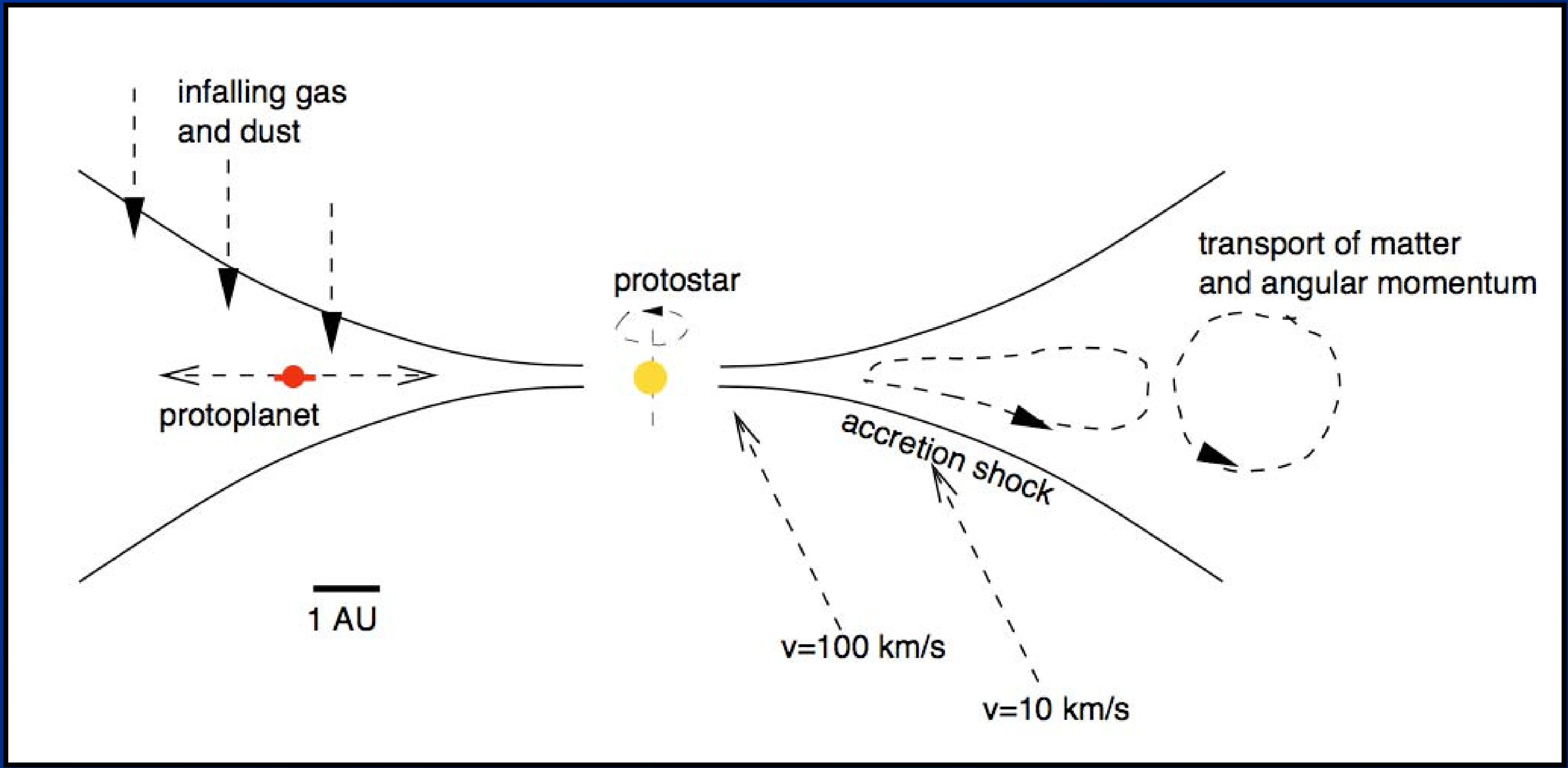
Models of Protoplanetary Disks



- stationary 2D disk models
- irradiation by the star (+ accretion) determines the disk structure

[Chiang & Goldreich 1997, D'Alessio et al. 1998, Willacy & Langer 2000, Aikawa et al 2002, Jonkheid et al. 2004, Kamp & Dullemond 2004, Nomura & Millar 2005, Meijerink et al. 2008]

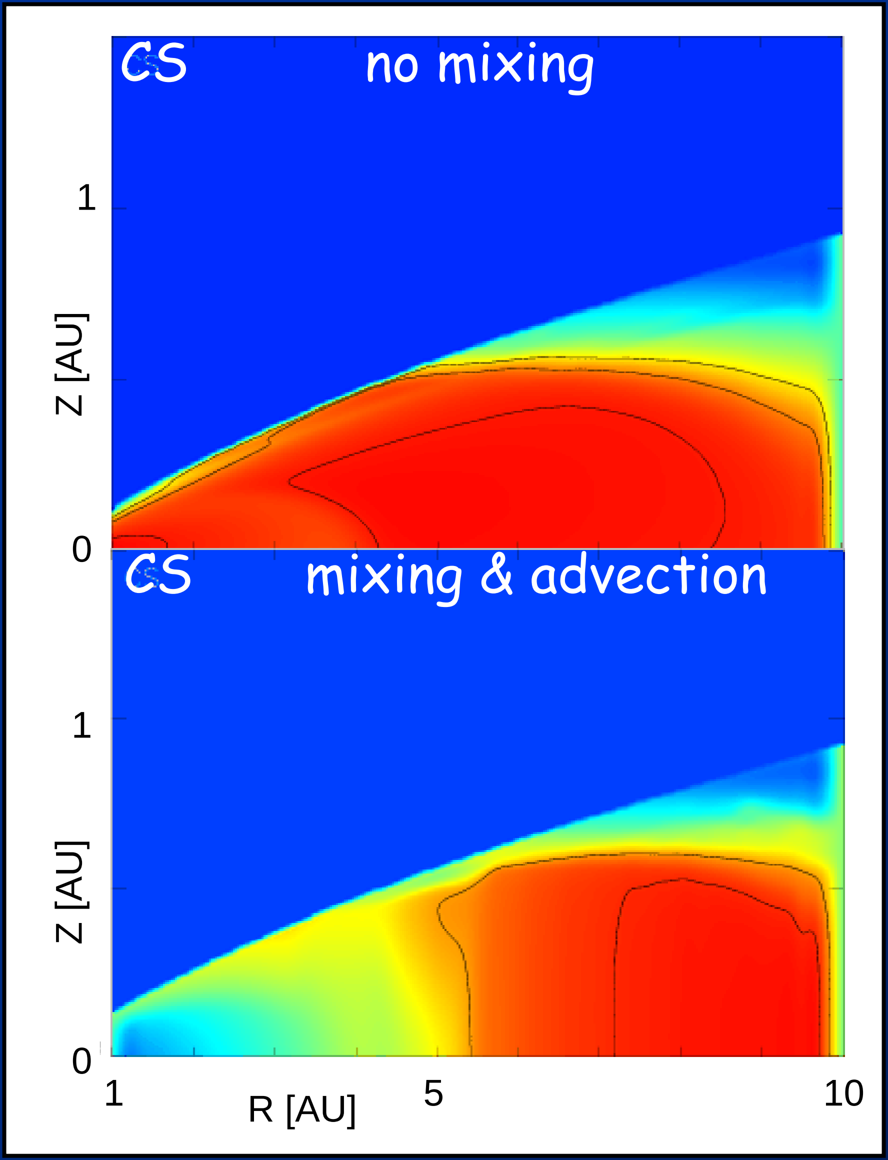
Models of Protoplanetary Disks



- matter is mixed and transported by turbulence
- matter accretes onto the central star $dM/dt \sim 10^{-7}\ M_{Sun}/yr$
- matter continuously falls in from the envelope causing an accretion shock at the disk surface

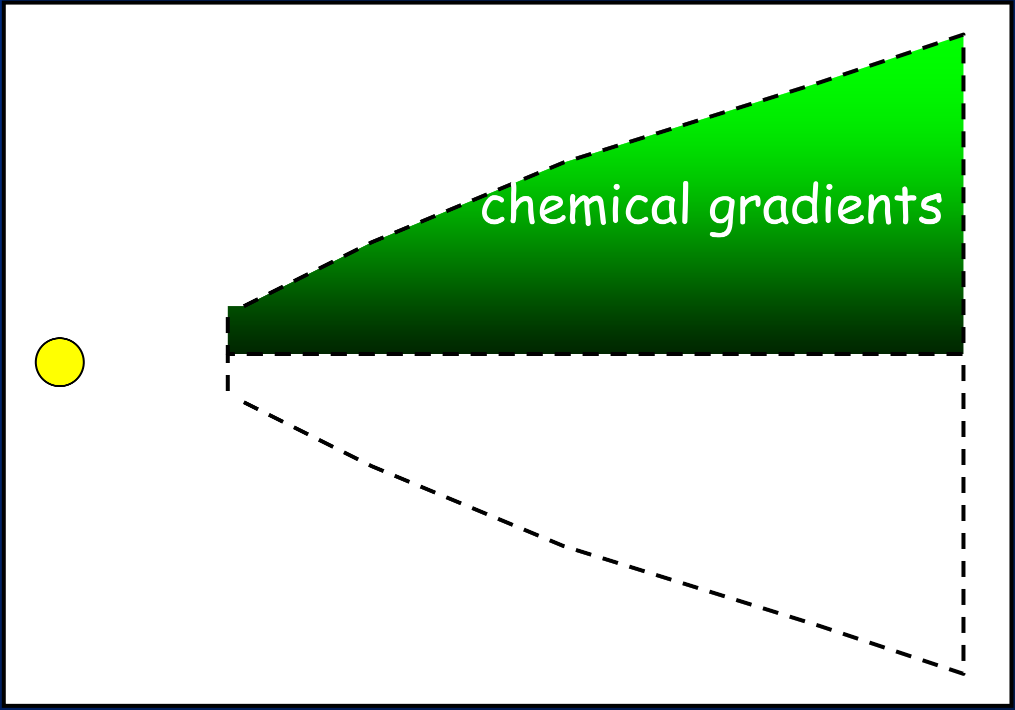
[Aikawa et al. 1999, Gail 2001, Ilgner et al. 2004, Willacy et al. 2006, Semenov et al. 2006]

How does mixing affect the chemistry?



[Ilgner et al. 2004]

Mixing has strong effects on the sulphur chemistry in the inner disk R < 10 AU.



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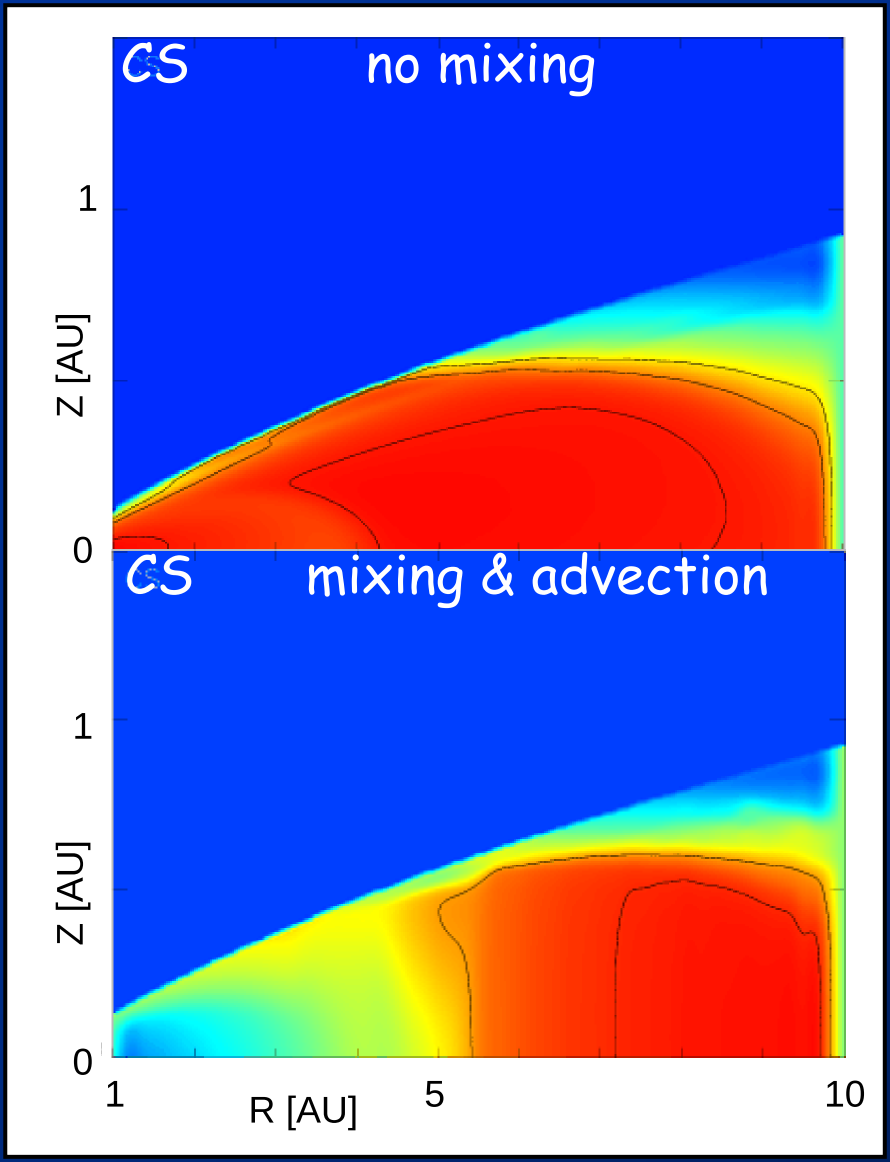

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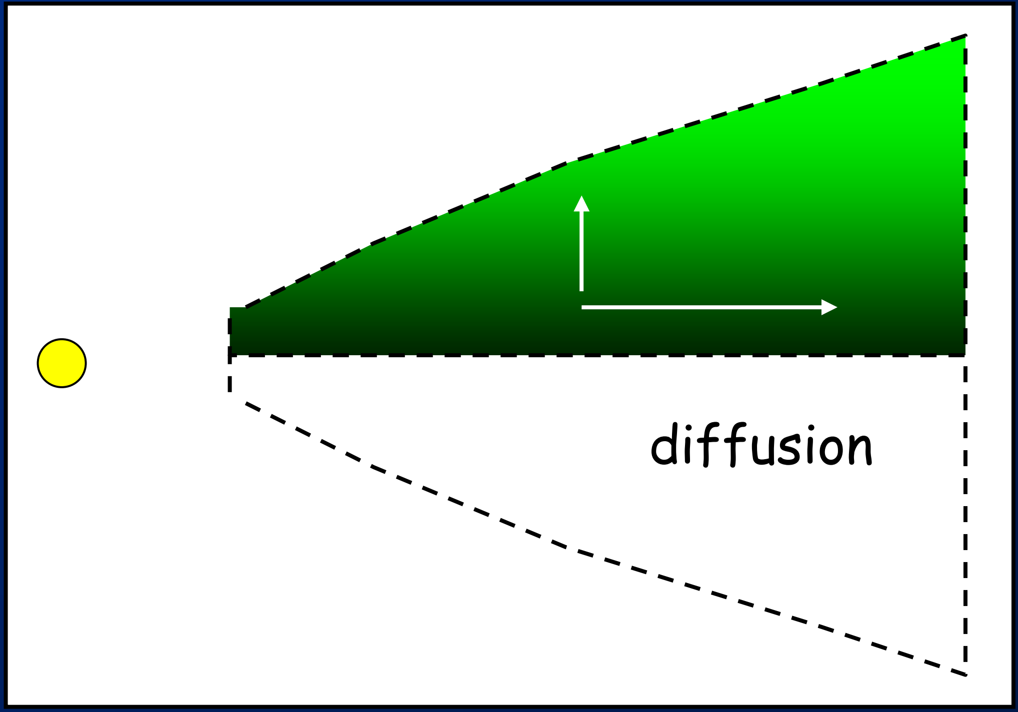

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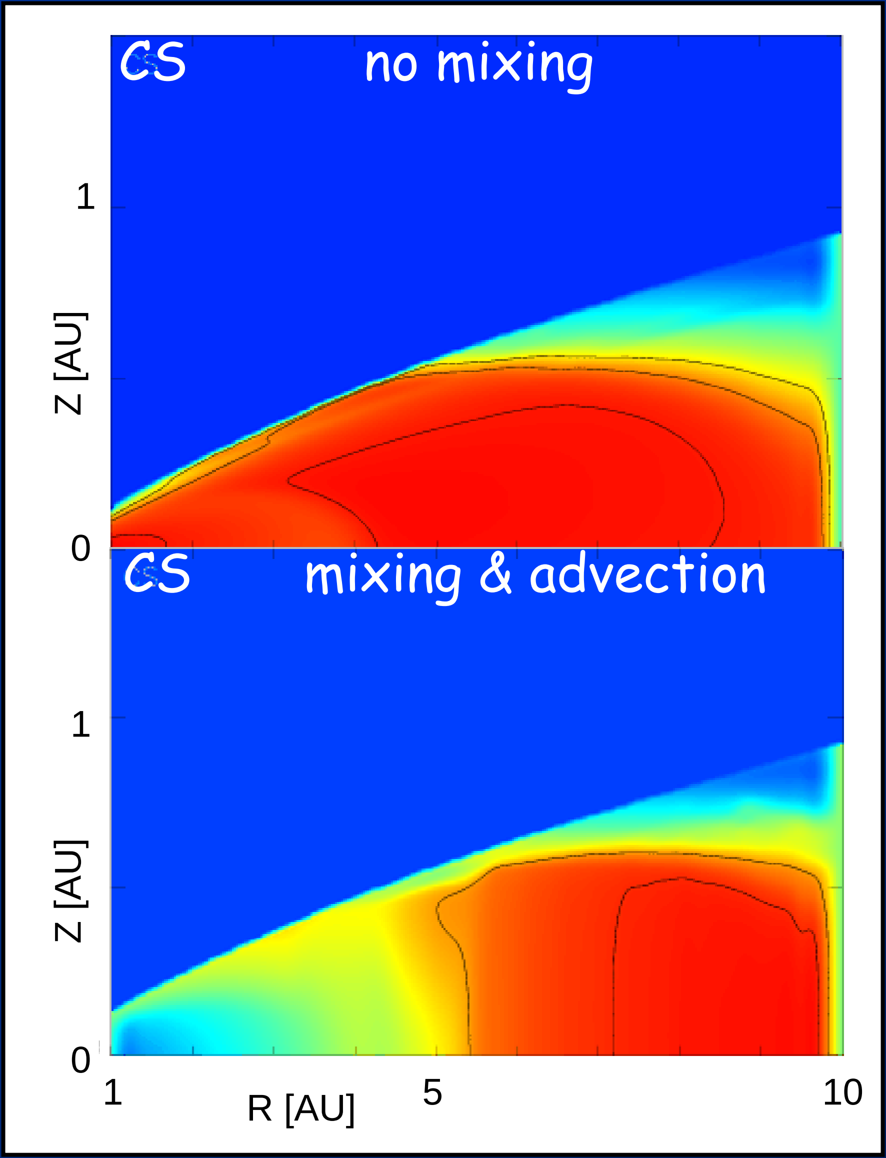

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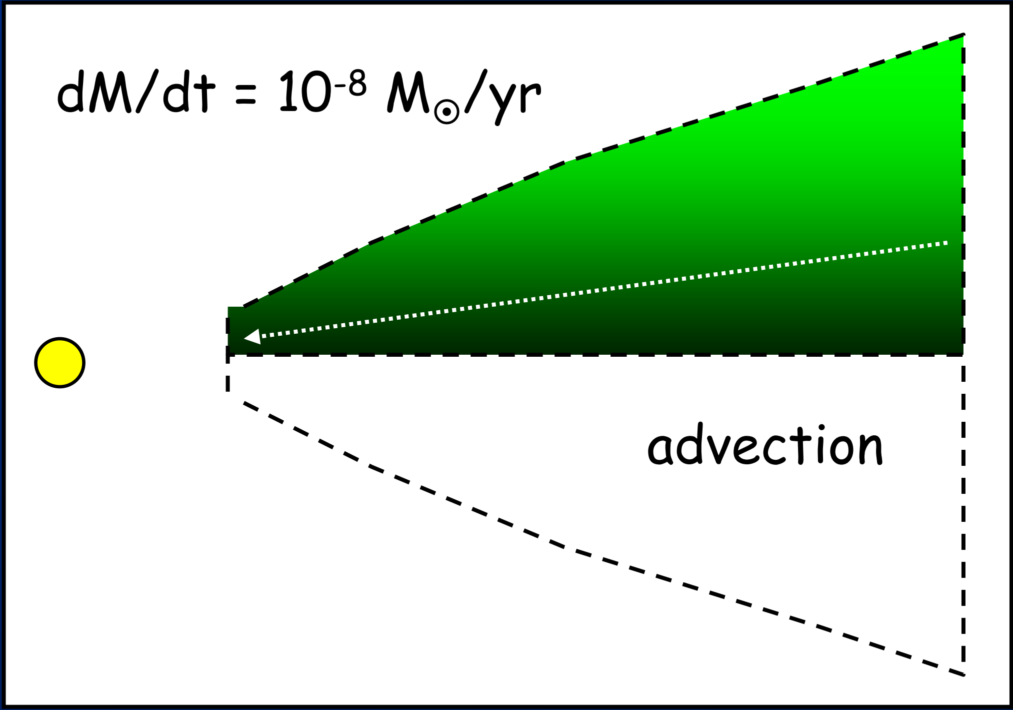

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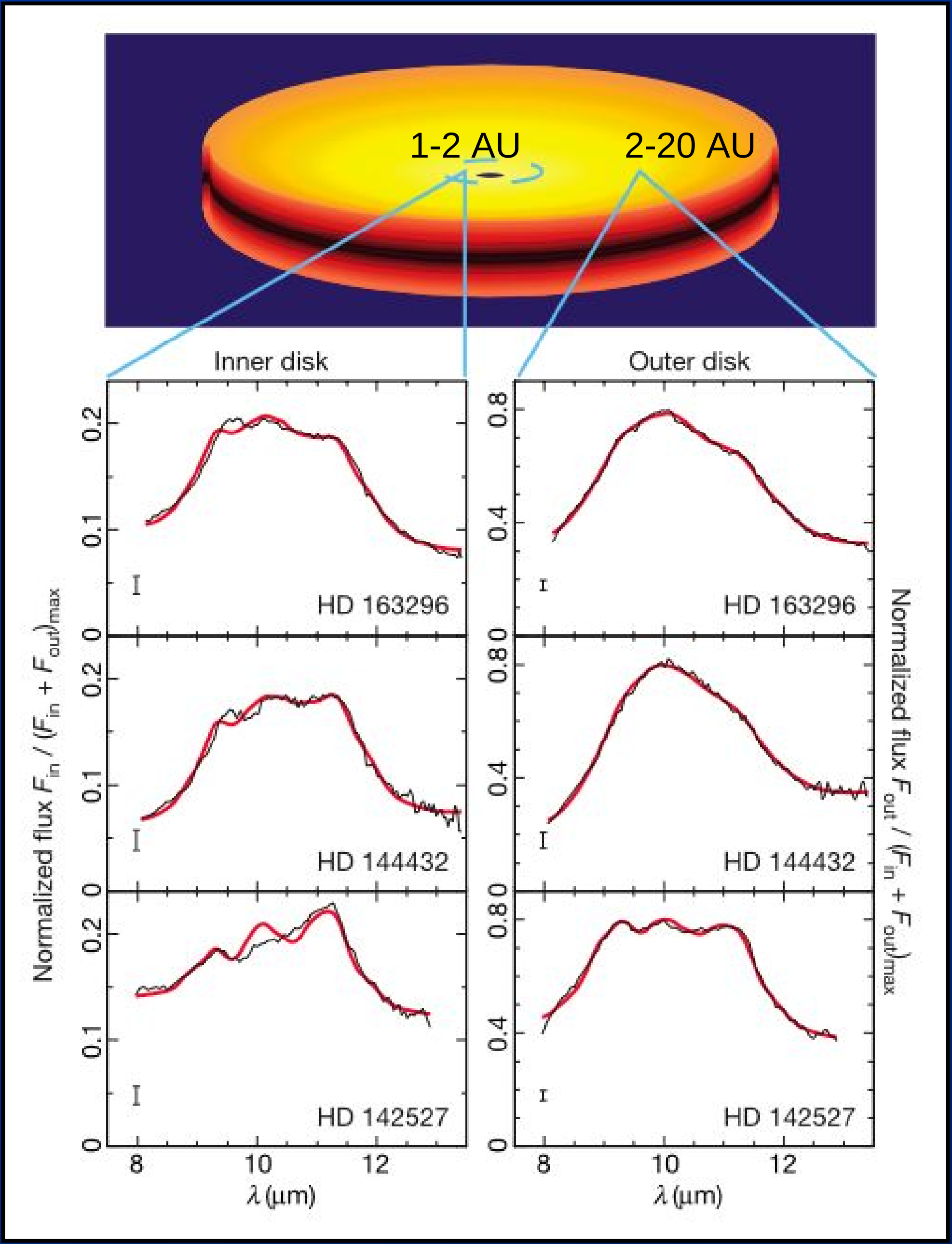
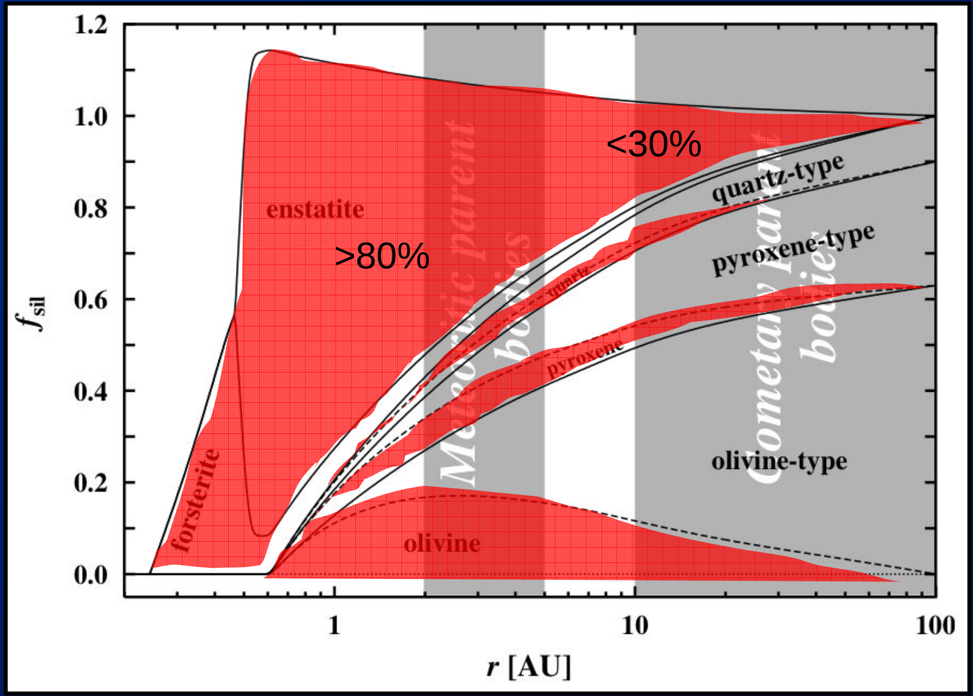


[van Boekel et al. 2004]

Inner disk has higher degree of crystallinity than outer disk.

Solid-gas chemical equilibrium models explain this with high temperatures and radial mixing.



[Gail 2004]