

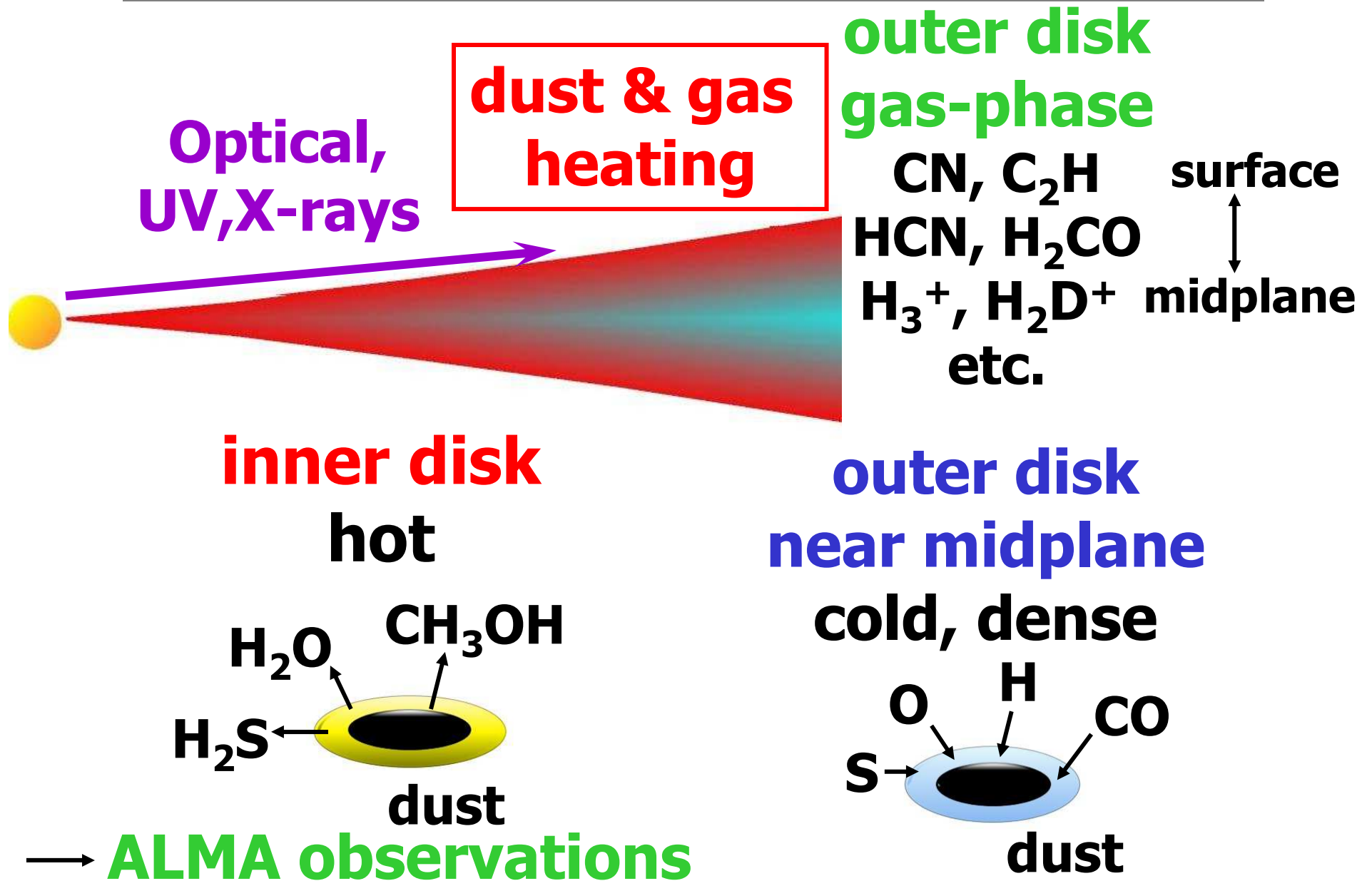
**Transformational Science with ALMA:
Through Disks to Stars and Planets**

Distributions of Hot Molecules in Young Circumstellar Disks

**Hideko Nomura¹, Yuri Aikawa²,
Yoshitsugu Nakagawa², Tom Millar¹**
1. Queen's University Belfast, 2. Kobe Univ.

1 Introduction

Chemical Structure of Young Disks

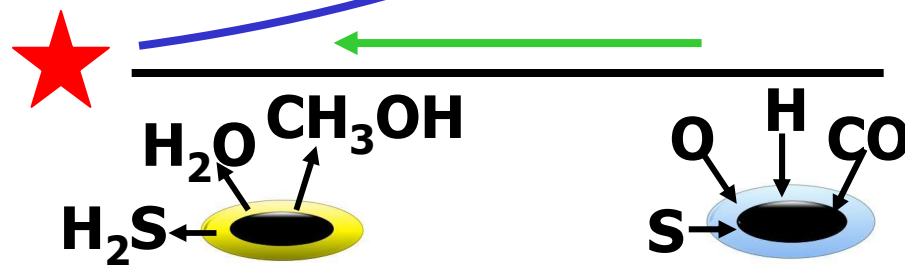


Disk Accretion & Chemistry

Disk Accretion:

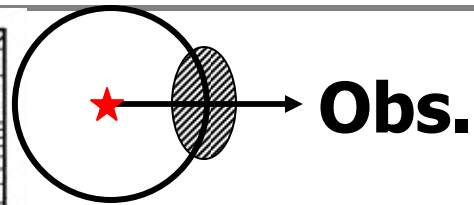
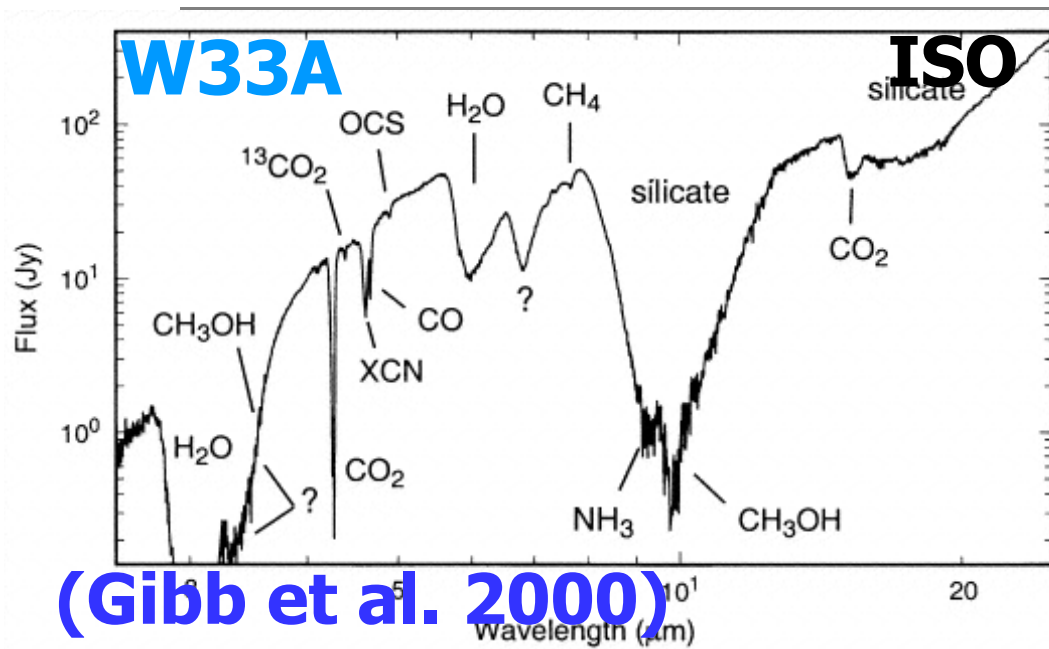
gas disk dispersal
gaseous planet formation,
migration of (proto)planets

↔ **Theory: MRI? Observation?**

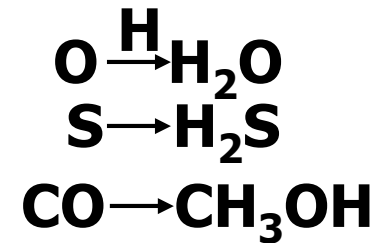
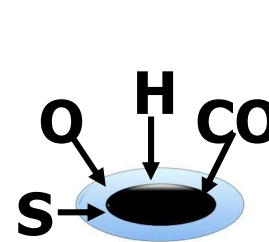


Icy mantle evaporation →
observational diagnosis of disk accretion?

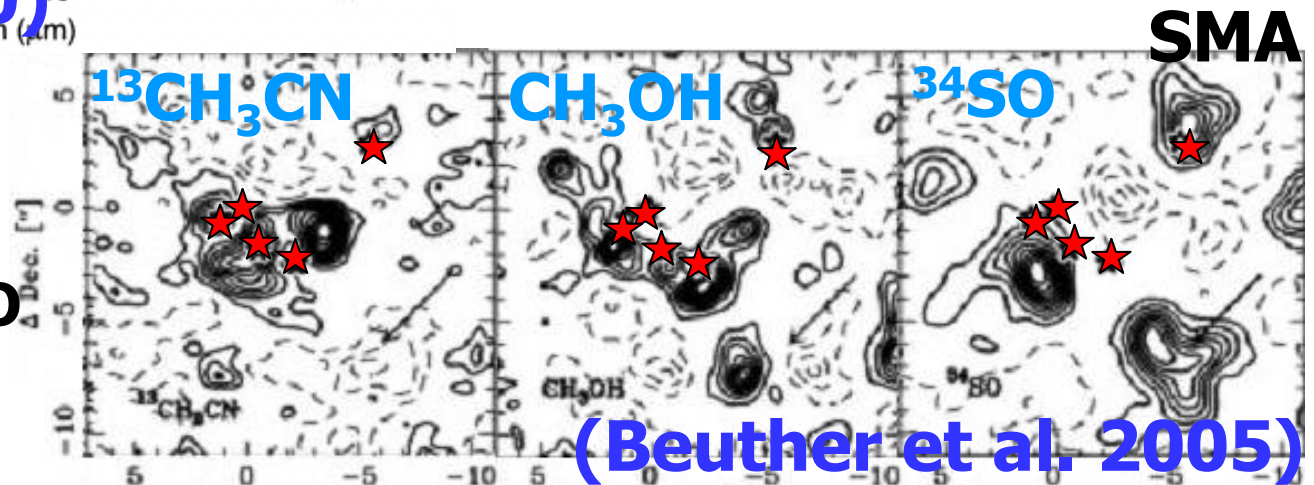
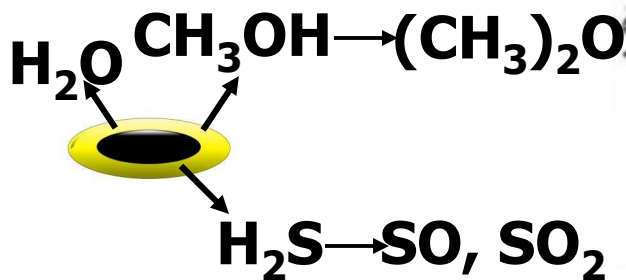
Obs. of Solid & Gas-Phase Molecules



cold, dense



hot



$\text{NH}_3, \text{H}_2\text{S}, \text{CH}_3\text{OH}, \text{HCN}, \text{SO}, \text{SO}_2, (\text{CH}_3)_2\text{O}$: abundant

Obs. of Molecular Abundances

Molecules	Orion Hot Core	AFGL 2591	TMC1
H ₂ O	1.0(-5)	3.6(-5)	
H ₂ S	≤ 5.0(-6)	≤ 1.0(-4)	2.5(-10)
SO	1.5(-7)	2.0(-8)	2.5(-9)
SO ₂	9.4(-8)	6.3(-7)	5.0(-10)
NH ₃	1-10(-6)	2.0(-8)	1.0(-8)
HNC	3.0(-7)	3.0(-7)	1.0(-8)
CH ₃ CN	7.8(-9)	2.0(-8)	5.0(-10)
CH ₃ OH	1.0(-6)	8.0(-8)	1.0(-9)

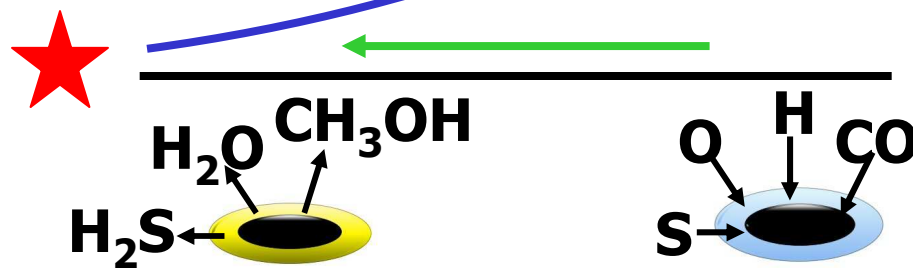
(from Charnley et al. '92, Charnley '97,
Ikeda et al. '01, Doty et al. '02, Lee et al. '96)

Disk Accretion & Chemistry

Disk Accretion:

gas disk dispersal
gaseous planet formation,
migration of (proto)planets

↔ Theory: MRI? Observation?



Icy mantle evaporation →
observational diagnosis of disk accretion?

2 Models

Gas, dust temp. & density profiles

gas dens.: hydrostatic equilibrium

($M_* = 2.5 M_s$)

surface dens.: steady accretion model

$$dM_{\text{acc}} = (0.5-20) \times 10^{-8} M_s / \text{yr} (= \text{const.})$$

gas temp.: local thermal equilibrium

Γ_x : X ray heat., Γ_{pe} : FUV heat., Λ_{line} :
radiative cooling, L_{gr} : gas-grain collisions

dust temp.: local radiative equilibrium

(irradiation($T_* = 10000\text{K}$), viscous heating)

dust dens.: coagulation equation

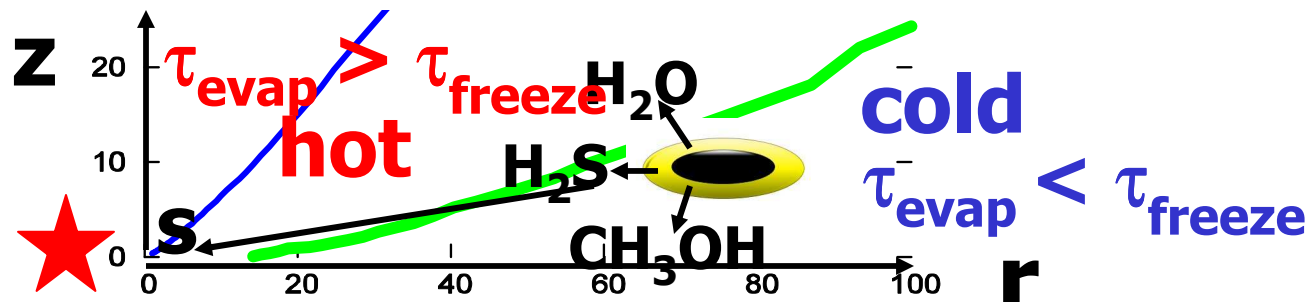
for settling dust particles

(Nomura et al. 2007)

Chemical Model

Chemical kinetic models

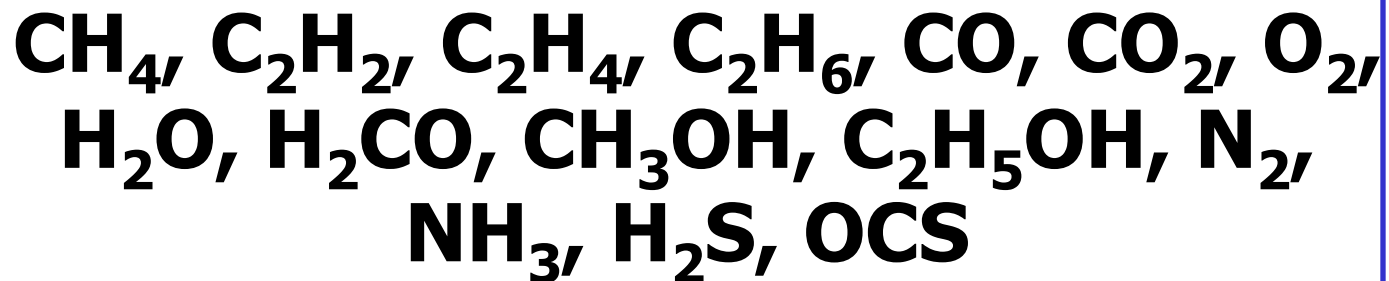
$$\frac{d(n_{\alpha} v_{\alpha})}{ds} = \sum_{\beta} A_{\alpha\beta} n_{\beta} + \sum_{\beta, \gamma} B_{\alpha\beta\gamma} n_{\beta} n_{\gamma}$$



Chemical reaction network :

209 species, 2203 gas-phase reactions

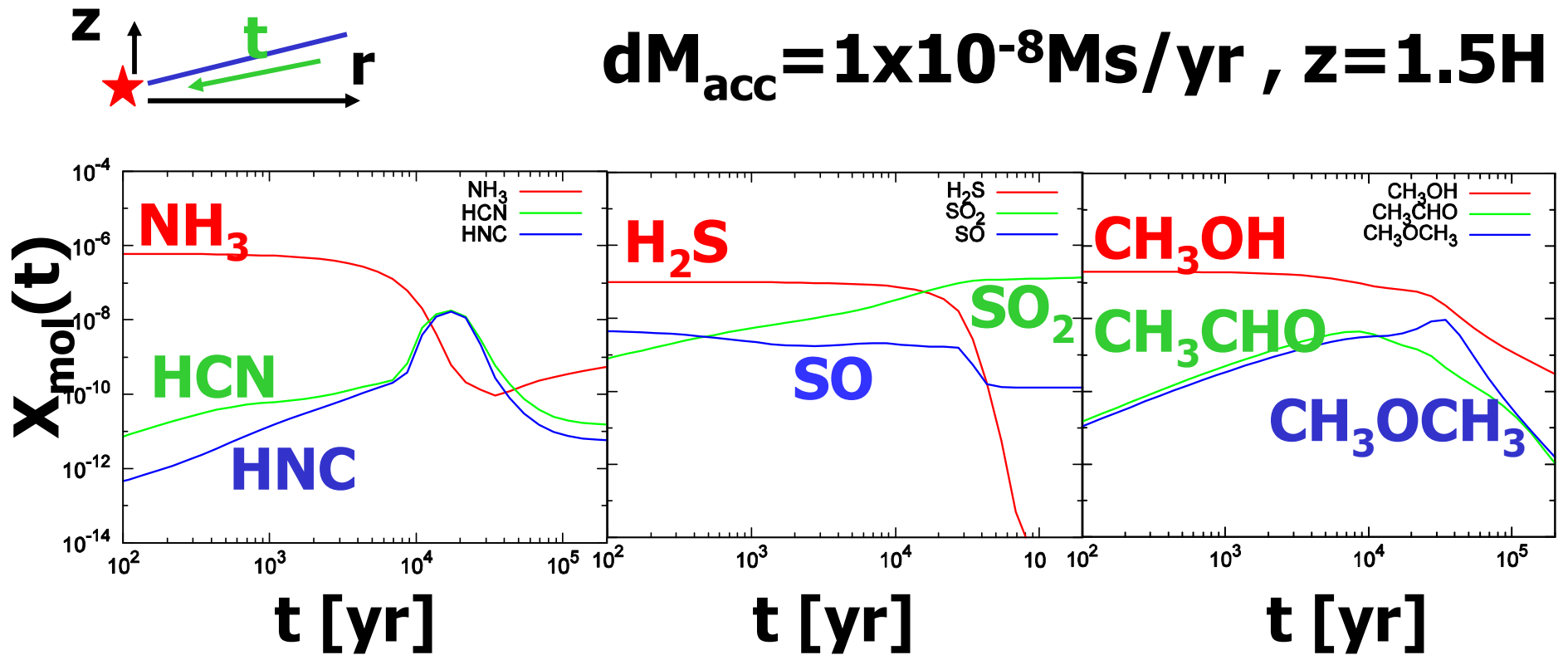
Initial condition: ice evaporation



(Nomura & Millar 2004)

3 Results

Time evolution of Mol. Abundances



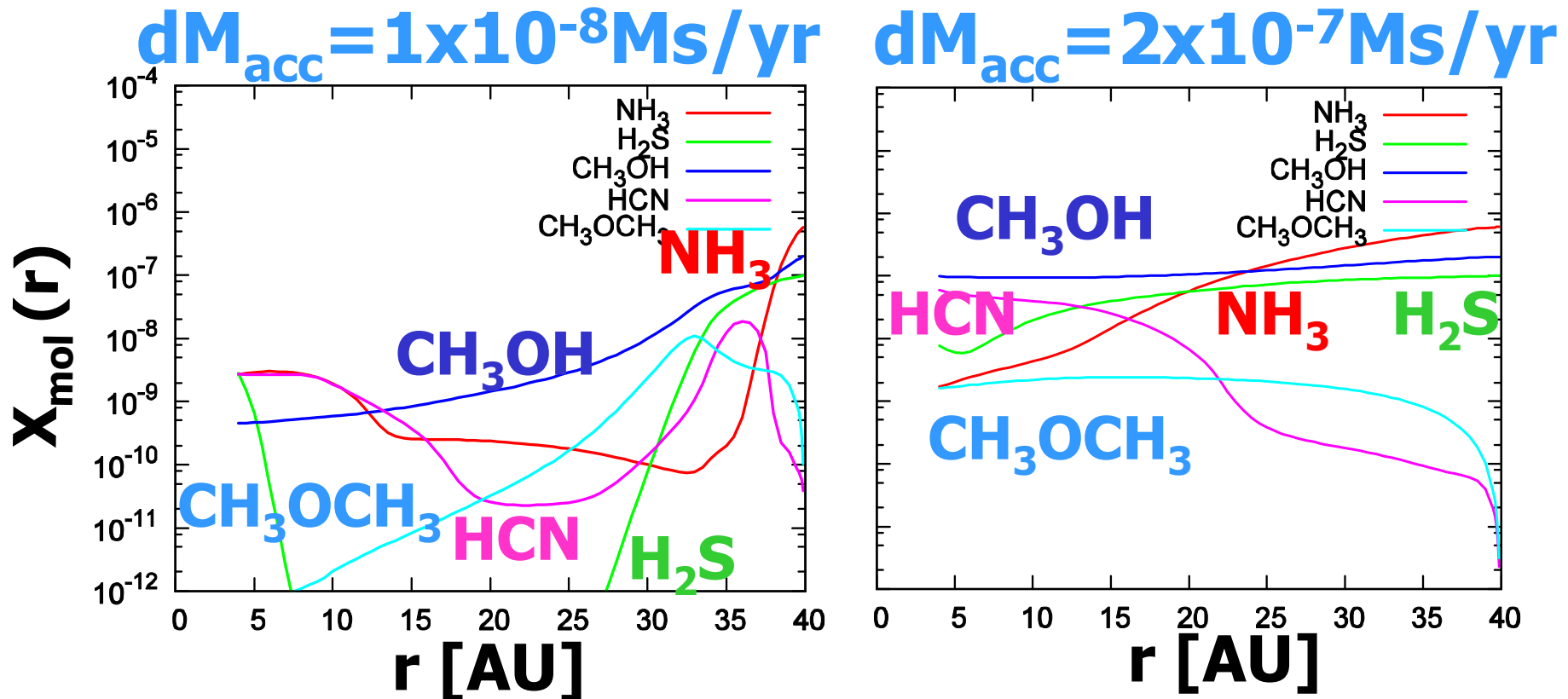
Parent species (CH₃OH, H₂S)

→ **Daughter species (CH₃OCH₃, SO₂ etc.)**

timescale : $t \sim 10^4 - 5 \text{ yr}$

Spatial Distributions of Molecules

$z=1.5H$



$dM_{\text{acc}} = 1 \times 10^{-8} \text{ Ms/yr}$ ($\tau_{\text{acc}} > \tau_{\text{react}}$)

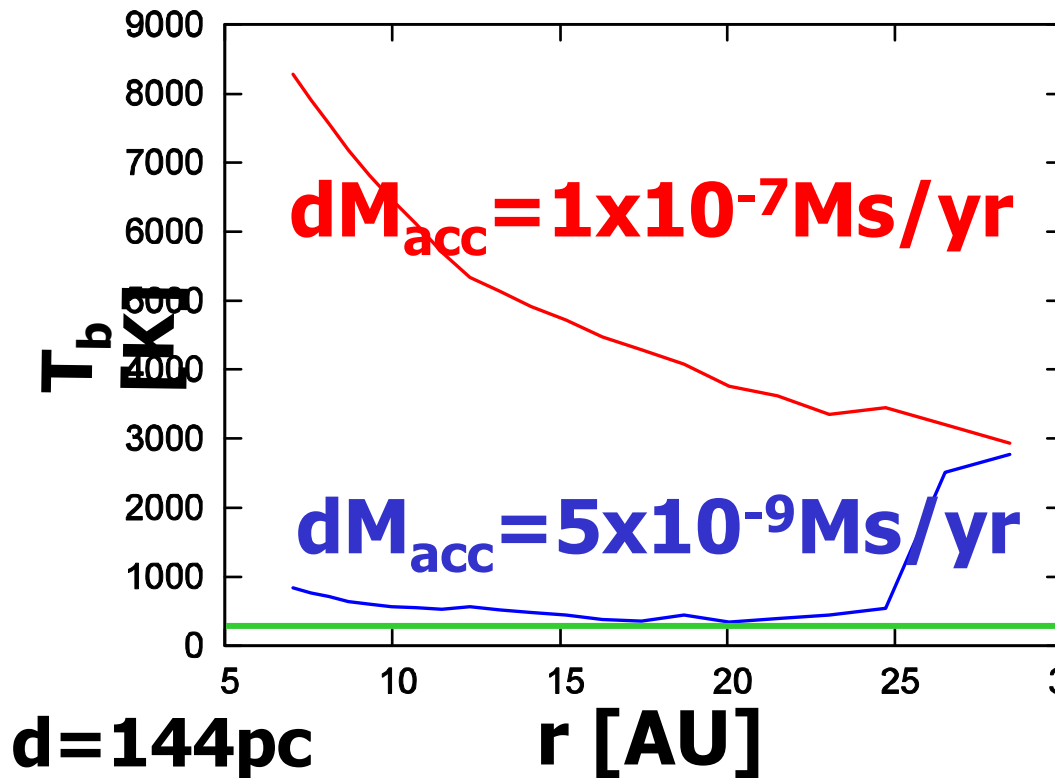
: high abundances only at large r

$dM_{\text{acc}} = 2 \times 10^{-7} \text{ Ms/yr}$ ($\tau_{\text{acc}} < \tau_{\text{react}}$)

: parents: uniform, daughter: high at inner

Spatial Distribution of Line emission

CH₃OH: J_K=7₋₁ → 6₋₁ @338GHz



$$F_{\text{ul},r} = \int_{-z_{\infty}}^{z_{\infty}} n_u A_{\text{ul}} \frac{h\nu_{\text{ul}}}{4\pi} \exp(-\tau_{\text{ul}}) dz$$

n_u : LTE distribution
(Hogerheijde & van der Tak 2000, Schoier et al. 2005)

ALMA 5 σ detections

10 antennas, 1km/s, 0".1, 600s

Dependence of spatial distribution of line emission on accretion rate

→ Observable by ALMA

Spatial Distribution of Line emission

$$F_{ul,obs} = \frac{1}{\pi \Theta_{beam}^2} \int 2\pi r F_{ul,r} \exp(-r^2/\Theta_{beam}^2) dr$$

CH₃OH: J_K=2₁→1₁@97GHz

Θ_{beam} = 12".5
(~1800AU)

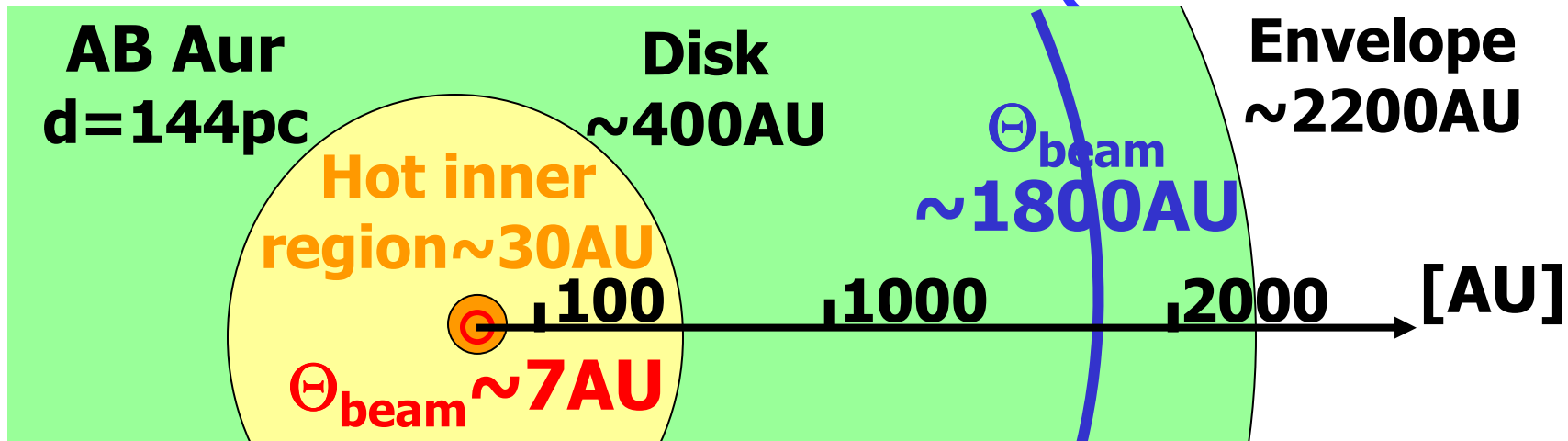
Θ_{beam} = 0".05
(~7AU)

T_b ~ 3.1mK (r < 30AU)

T_b ~ 130K

↔ **Non-detection**
with IRAM30m

Beam dilution effect
(Semenov et al. 2005)



4 Summary

Distribution of hot molecules in inner region of young circumstellar disks

(evap. of ice + gas-phase reactions)

Timescale of chemical reactions: $\sim 10^{4-5}\text{yr}$

accretion time $> 10^{4-5}\text{yr}$

→ high abundances only at large r

accretion time $< 10^{4-5}\text{yr}$

→ parents: uniform, daughter: high at inner

Dependence of accretion rate on spatial distribution of line intensity

→ Observable by ALMA ?



Chemical Model

Initial Condition

Inject mantle molecules into gas

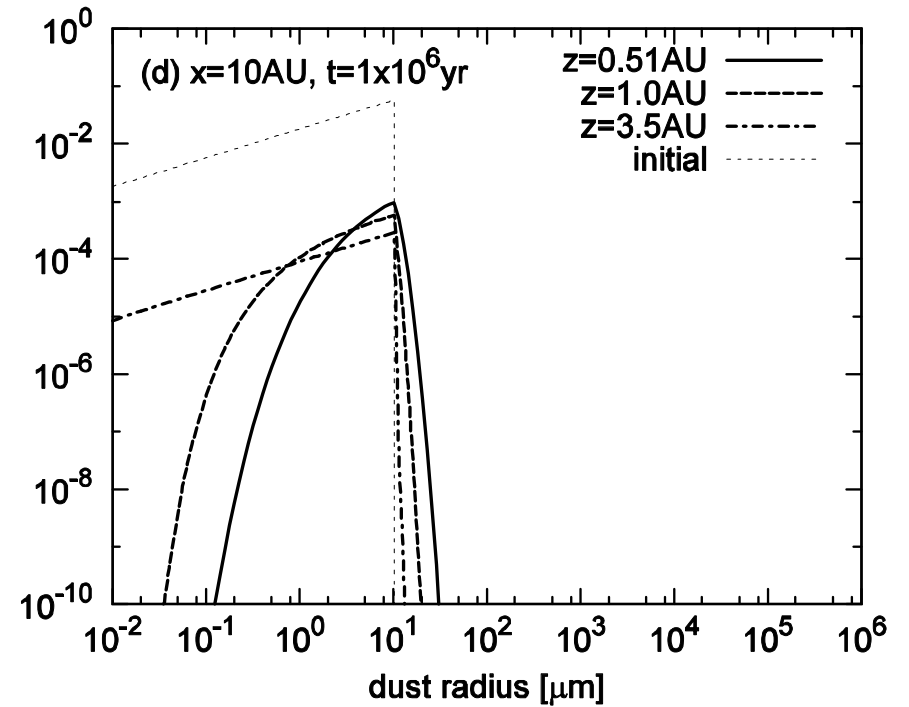
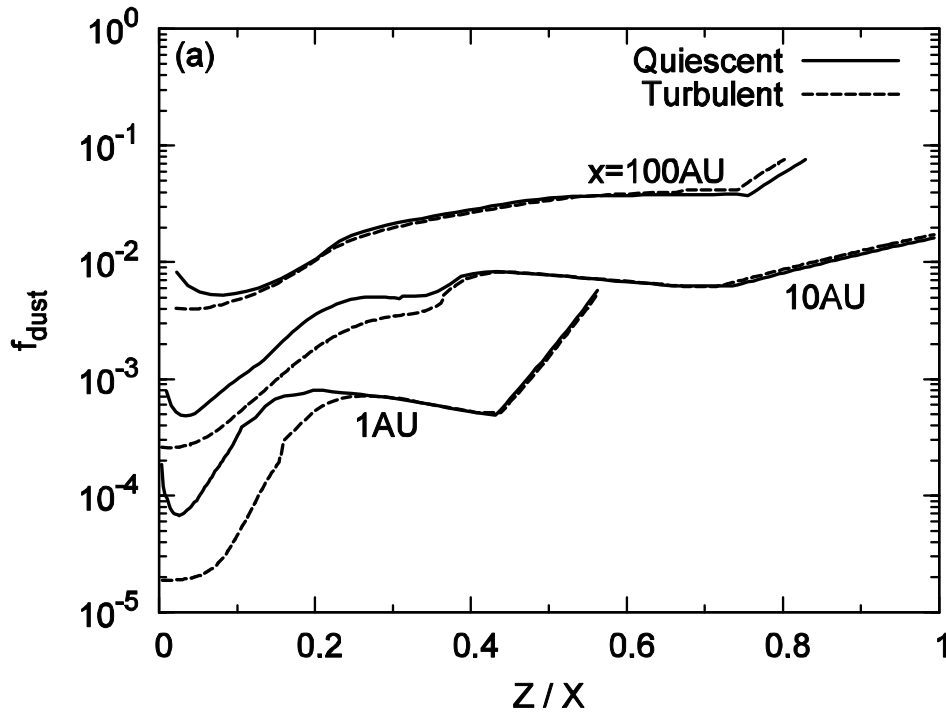
if $\tau_{\text{evap}, i} < \tau_{\text{freeze}, i}$;

$$\tau_{\text{evap}, i} = v_{0,i}^{-1} \exp(E_{b,i}/kT_d)$$

$E_{b,i}$: binding energy

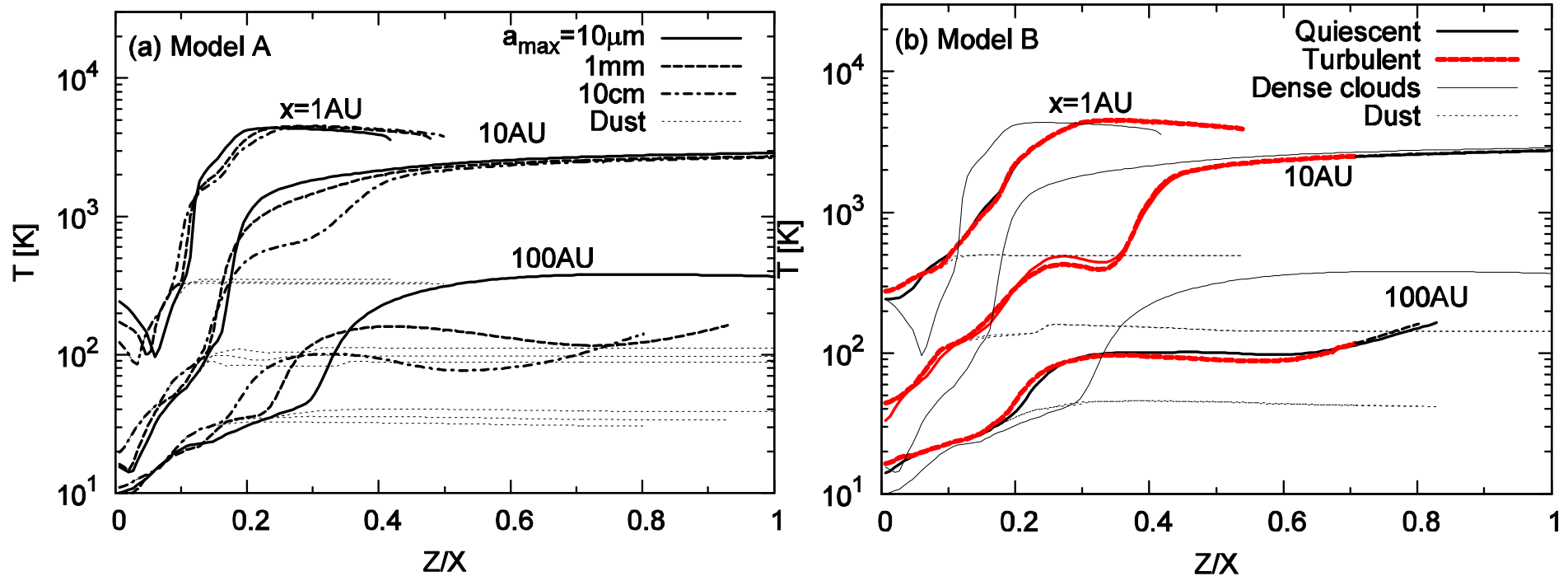
$$\tau_{\text{freeze}, i} = (S\pi a^2 d_g n v_i)^{-1} \\ \sim 10^9 \text{ yr} / n [\text{cm}^{-3}]$$

Dust Distribution



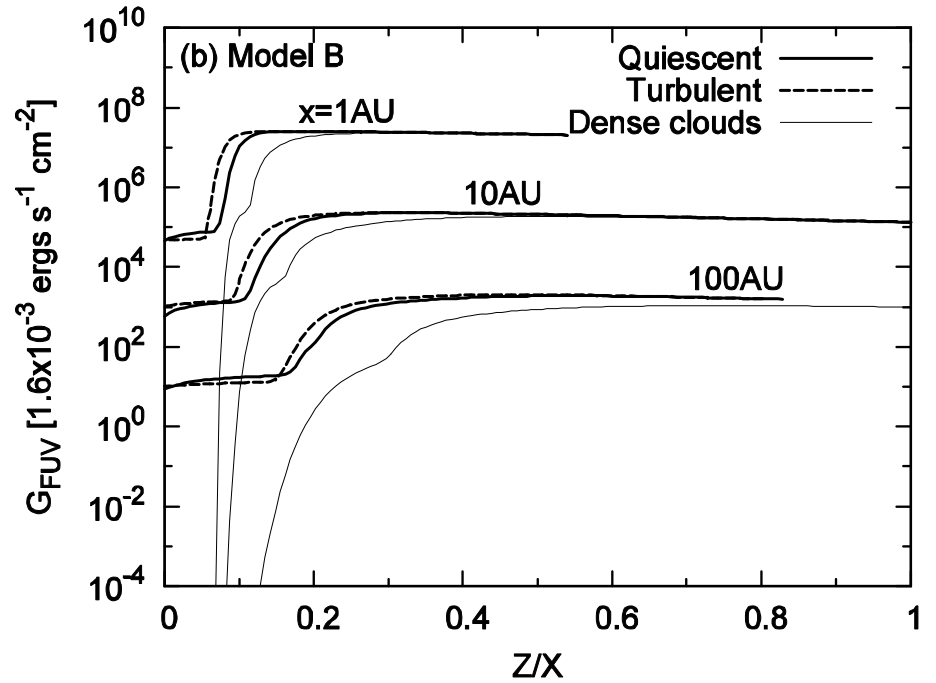
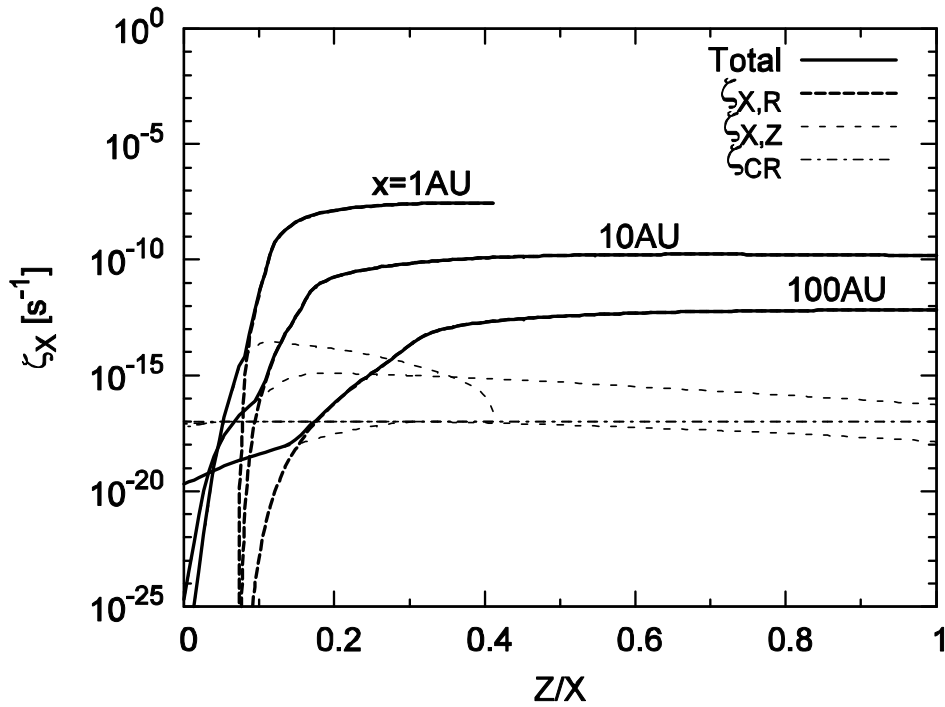
(Nomura et al. 2007)

Temperature Profiles



(Nomura et al. 2007)

X-rays & UV radiation fields

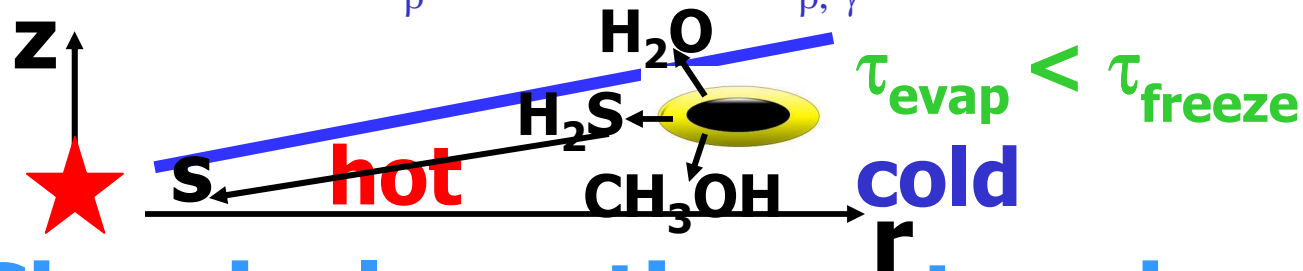


(Nomura et al. 2007)

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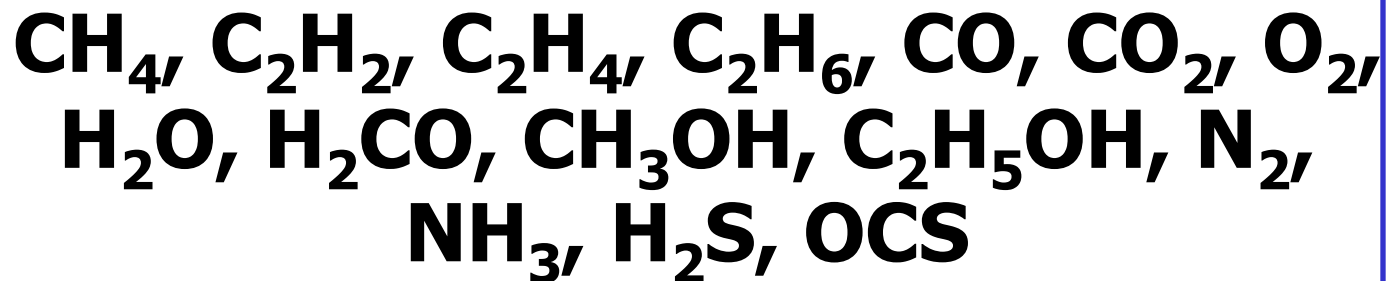
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