Disk Chemistry

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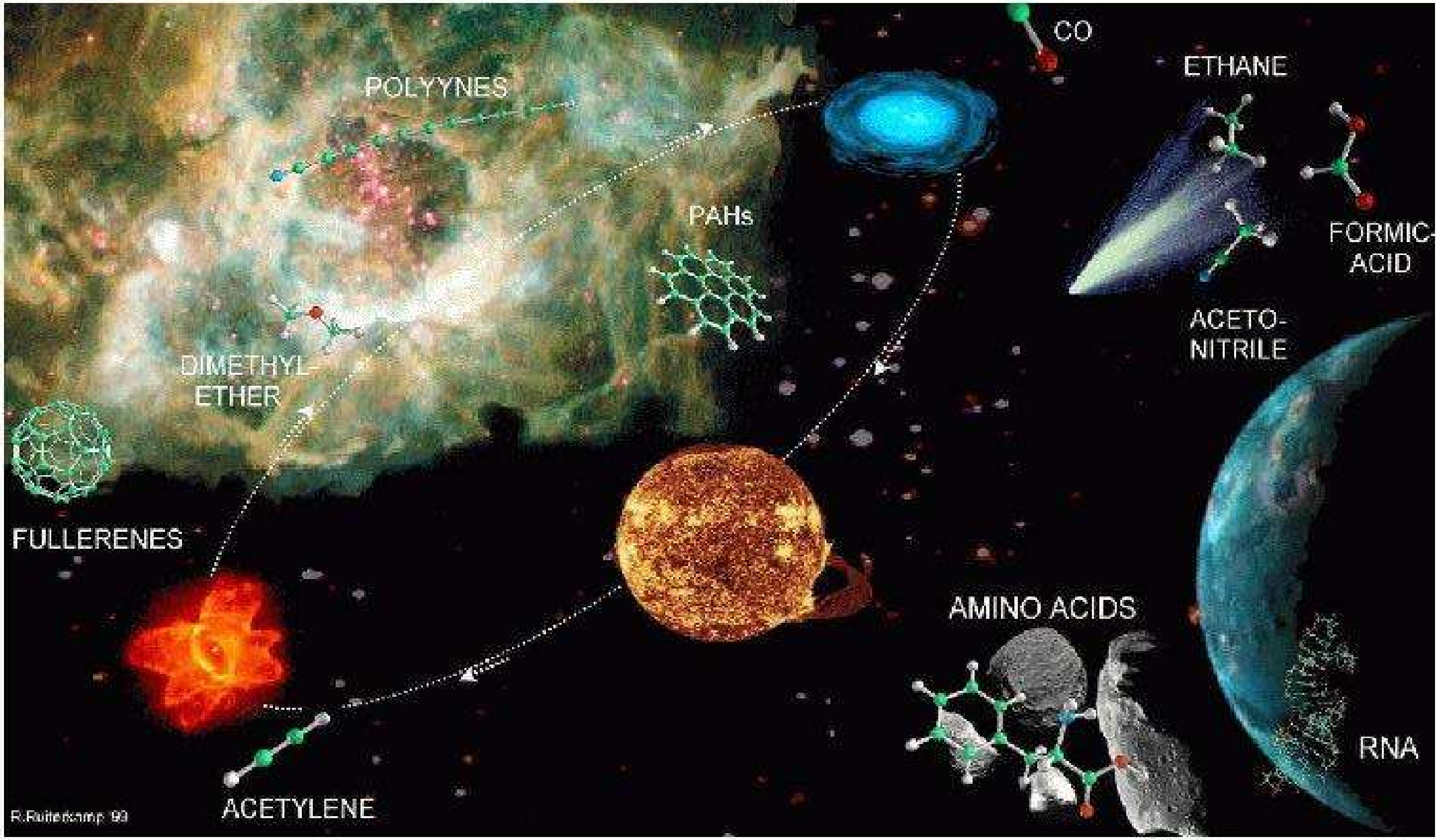

Protoplanetary Disks

Thin accretion disks from which protostar forms

Inflow from large radii (100 AU) onto central protostar

Temperature of outer disk is cold (10 K)

$n(H_2) \sim 10^{10} – 10^{15}$ cm^{-3}

Molecular gas is frozen on to dust grains in outer disk

Temperature of inner disk is ~ 100 K at 10 AU, ~1000 K at 1 AU

Ices evaporate in inner disk

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Chemical Processes

Ionization – X-rays, UV photons (direct + scatttered + IS), CRPs, CR-induced photons, radionuclides

Ion-neutral

Neutral-neutral

Two-body and three-body

Gas-Grain interaction – accretion, surface chemistry, evaporation, mutual neutralisation

Photodissociation – lines and continuum – photoionization

Physical Processes

UV radiative transfer in 2D

H_2 self-shielding, C^+/C/CO transition

UV excess ? Lyman alpha ?

Grain opacity

composition, size distribution

Gas cooling – O, C^+, C, CO

Dust heating/cooling – photoelectric emission

gas-grain collisions

Time-dependent or steady-state chemistry ?

Stellar heating ?

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Dust model

Dust properties affect

- UV intensity – absorption + scattering
- Grain temperature – re-processing stellar radiation
- Gas temperature – grain photoelectric heating and gas-grain collisions
- H/H_2 ratio – grain formation of H_2
- Excitation of H_2 on formation

Silicates, carbonaceous grains, water ice

Size distribution from Weingartner & Draine, MRN

Dust coagulation and settling

Initial Conditions

Steady state disk structure

Molecular cloud abundances – gas and ices

Effects of accretion shock ?

Temperature profile

models have midplane temperatures which range from 1500 K (Finocchi et al) to 680 K (Markwick et al) to 280 K (Aikawa et al) at 1 AU

Radiation field – Scaled IS, BB or T Tau stellar ?

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Chemical models

Early – 1996-1999

- One dimensional; Hayashi minimum solar mass, semi-analytic, Bell et al
- Gas-grain interaction not always included

Middle – 1999-2003

- 1 + 1 dimensions; Goldreich & Chang; D'Alessio, Bell et al
- Gas-grain interaction always included
- Ionization by UV, X-rays, CRs, radionuclides

Late – 2003-present

- 1 +1 dimensions - at 2500 grid points inside 10 AU
- Transport included; radial mixing, vertical diffusion
- Lyman alpha radiation
- Non-stationary disks
- Calculation of emergent line profiles

UV radiation

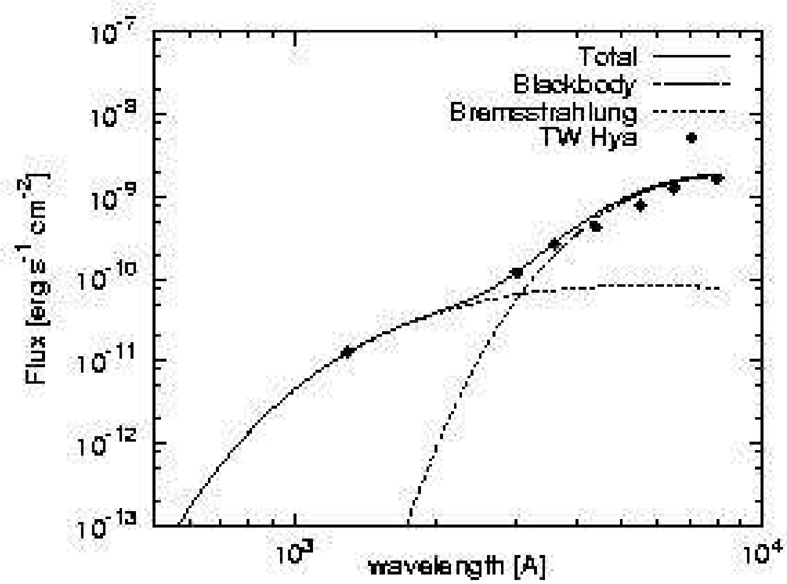
1 + 1 dimensional field

Radiation from central star – radial direction

IS radiation field + scattered stellar radiation – vertical direction

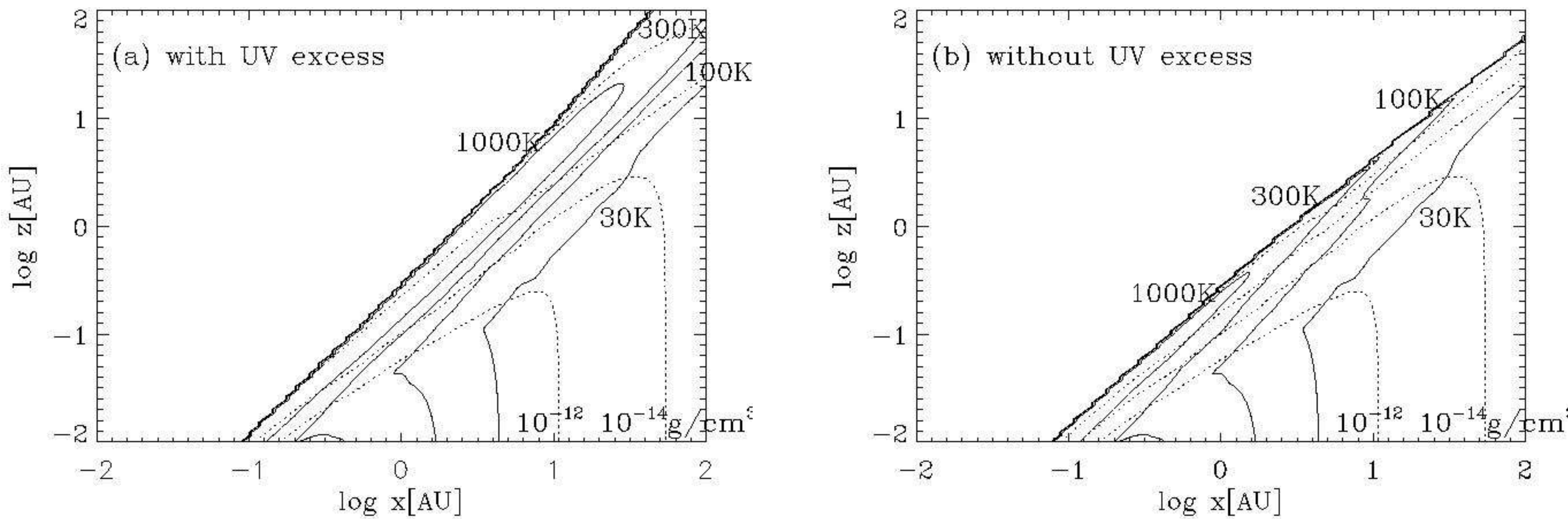
Over-estimates the true UV field

UV excess – adopted optically thin free-free radiation from fit to spectrum of TW Hya



Density and temperature profiles

Hotter surface layer
Thicker disk



Some processes – deuterium fractionation, freeze-out,
thermal desorption – very sensitive to low T regime
Some processes – H_2 reactions – very sensitive to high T regime

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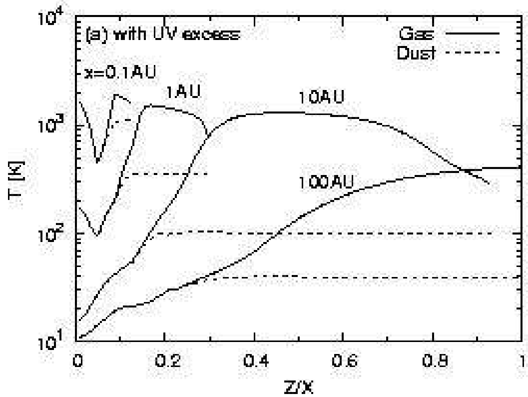
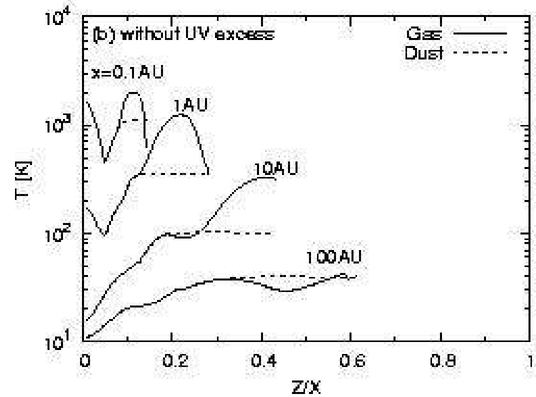
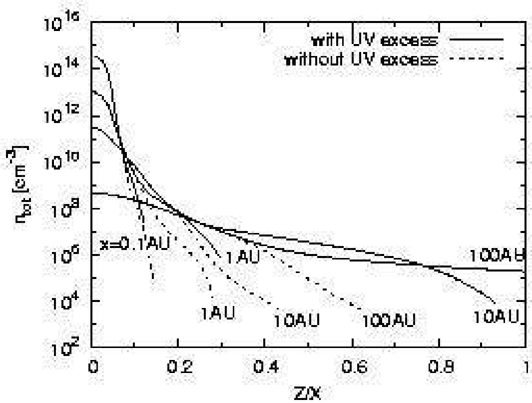
Vertical temperature distribution





UV excess causes greater p.e. heating, and temperatures of about 1000K at the surface

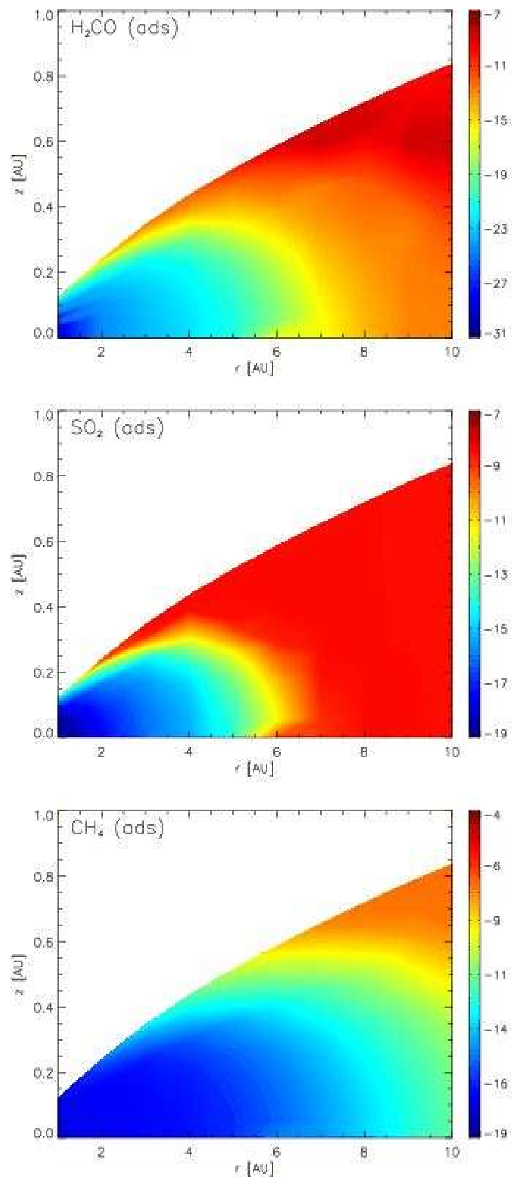


Density distribution

Heating causes expansion of disk vertically

Dust and gas temperatures decouple

Molecular Ice Distributions



Initial conditions taken
From dark interstellar
cloud model – with
freeze-out

Time-dependent chemistry
calculated at about 2500
grid points inside 10 AU

Markwick, Ilgner, Millar, Henning,
Astron. Astrophys., 385, 632 (2002)

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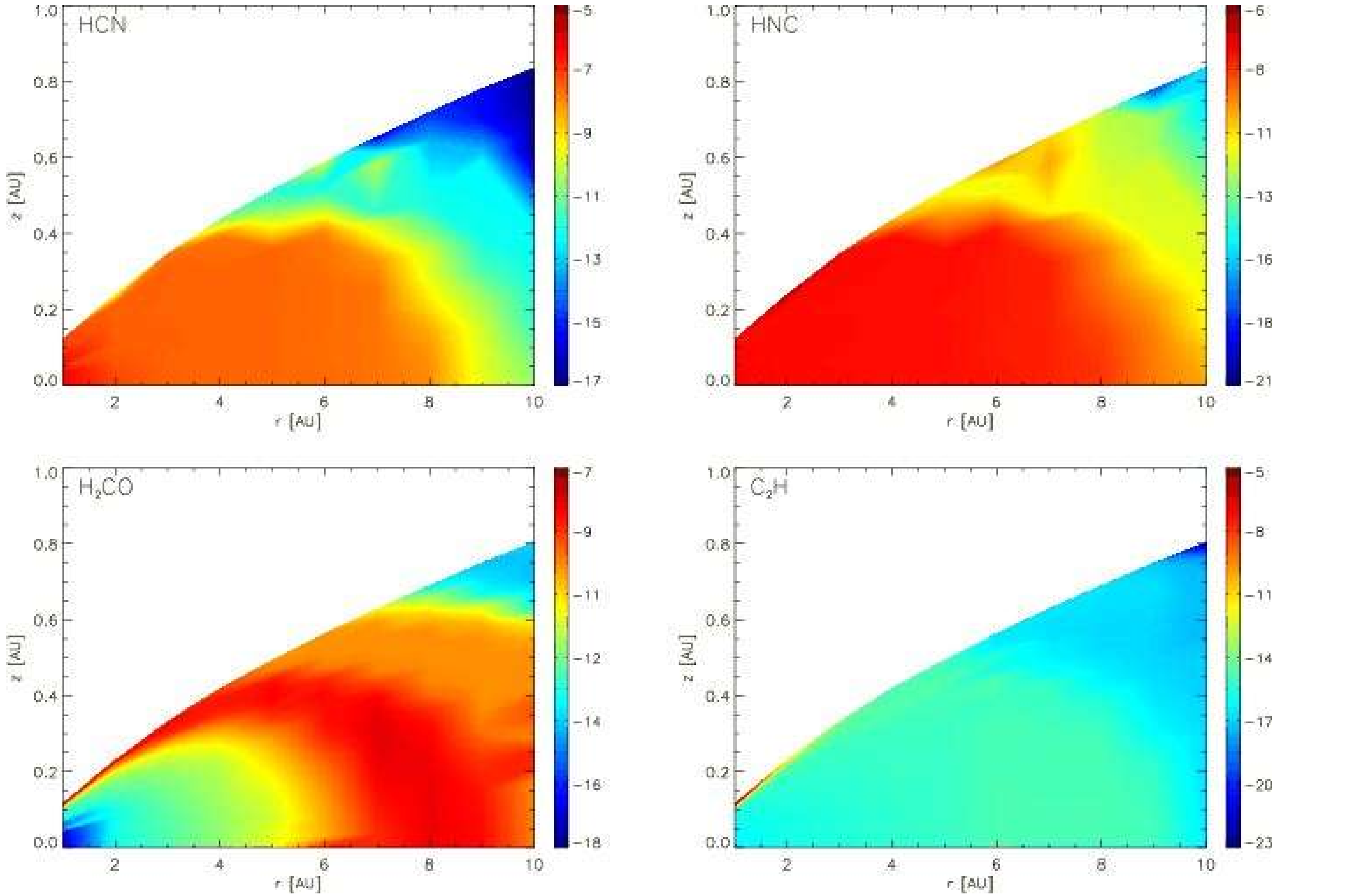
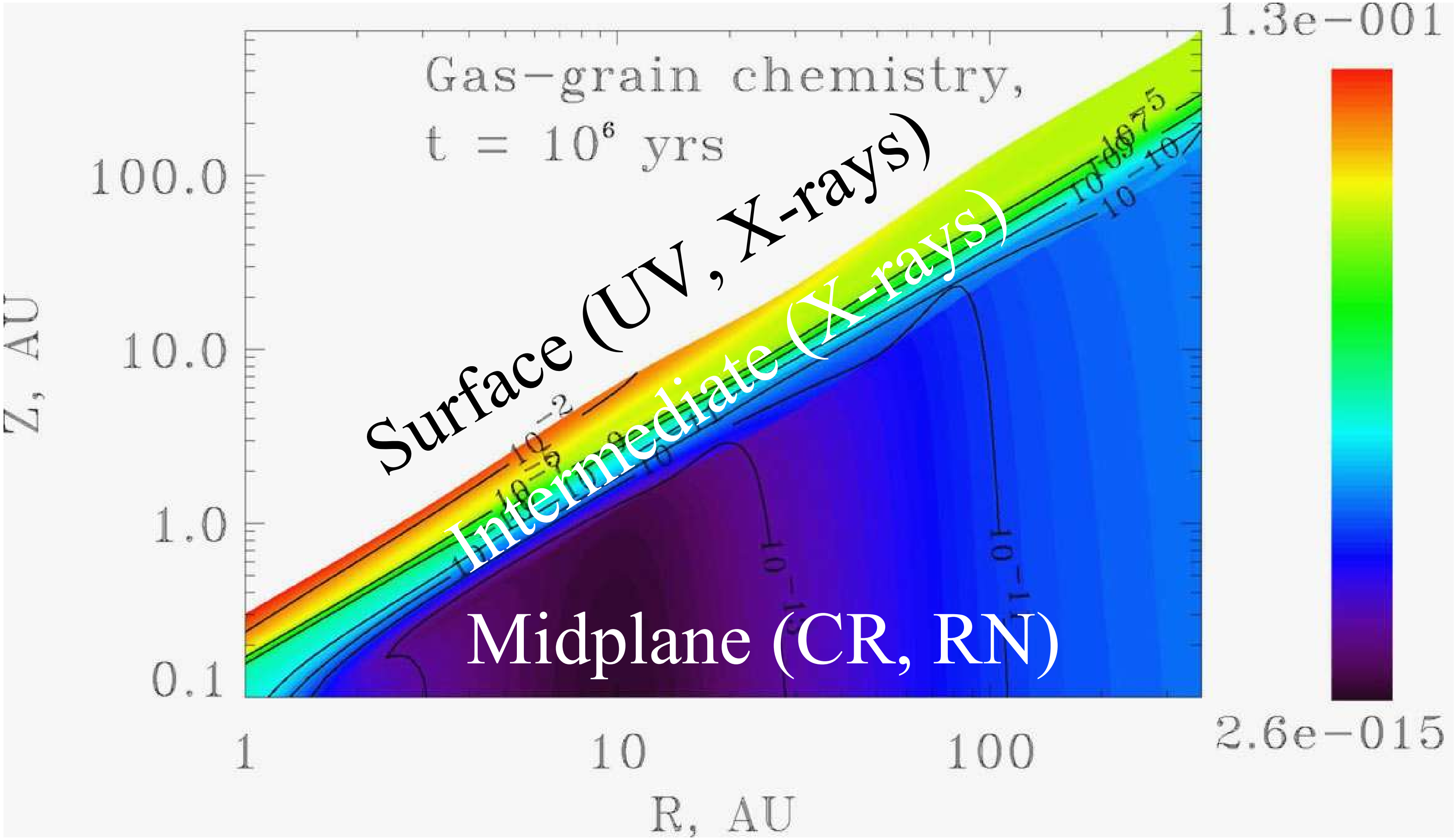
Molecular Distributions



Markwick, Ilgner, Millar, Henning, Astron. Astrophys., 385, 632 (2002)

Disk ionization degree at 1 Myr



Semenov, Wiebe, Henning

Chemical differentiation in *z*-direction

Surface layer (hot):

PDR-like chemistry (X-rays and UV),

H^+, He^+, C^+, CN, C_2H

Intermediate layer (warm):

Rich molecular chemistry (X-rays), surface reactions, desorption,

CS, CO, NH_3, H_2CO, HCO^+, $HCNH^+$, NH_4^+, H_3CO^+, S^+, He^+

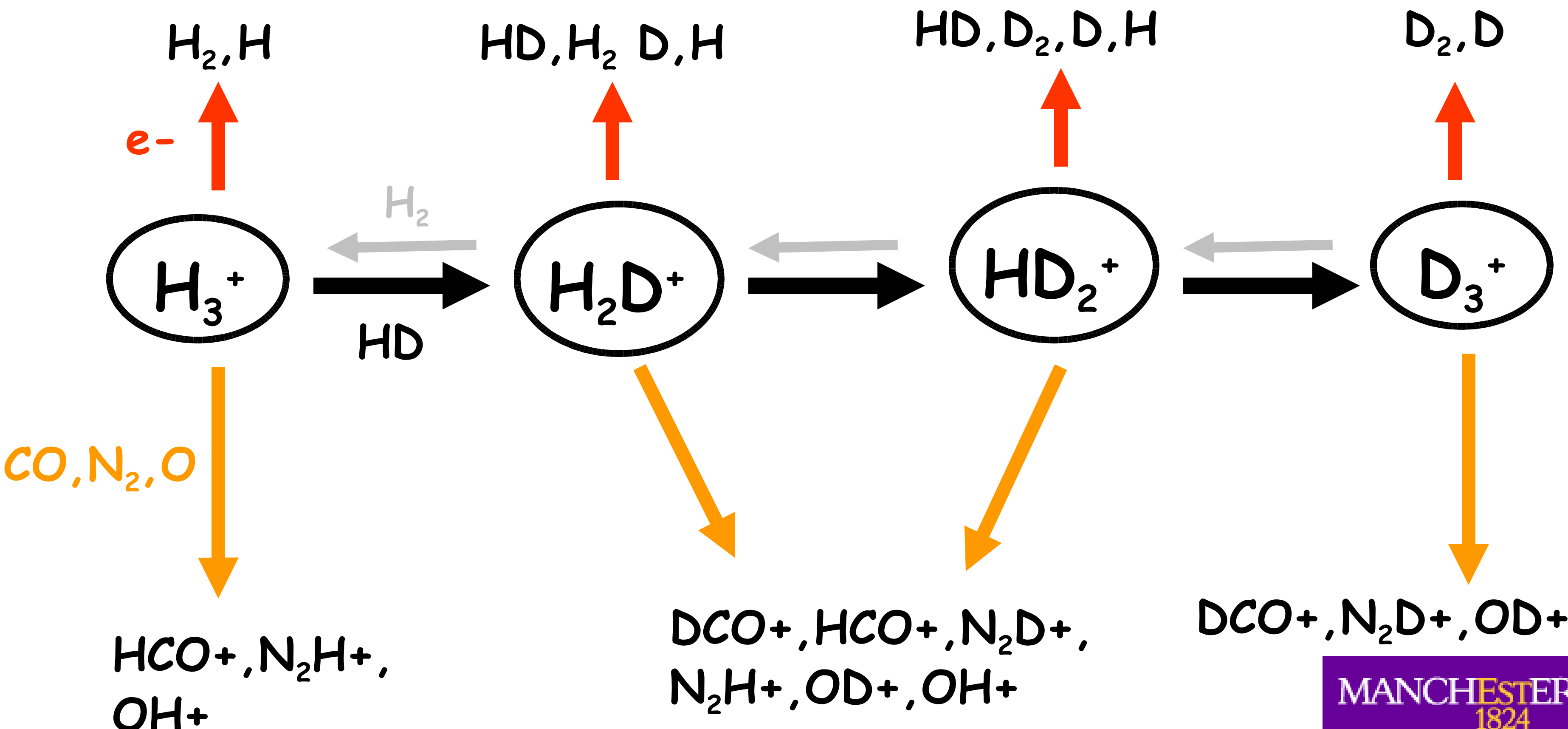
Midplane (cold):

Dark chemistry (CR and RN), 'total' freeze out,

Metal ions, H_3^+, HCO^+, N_2H^+ , H_2D^+, D_2H^+, D_3^+

Cold, depleted gas drives multiple deuteration

(See poster by Dominik)



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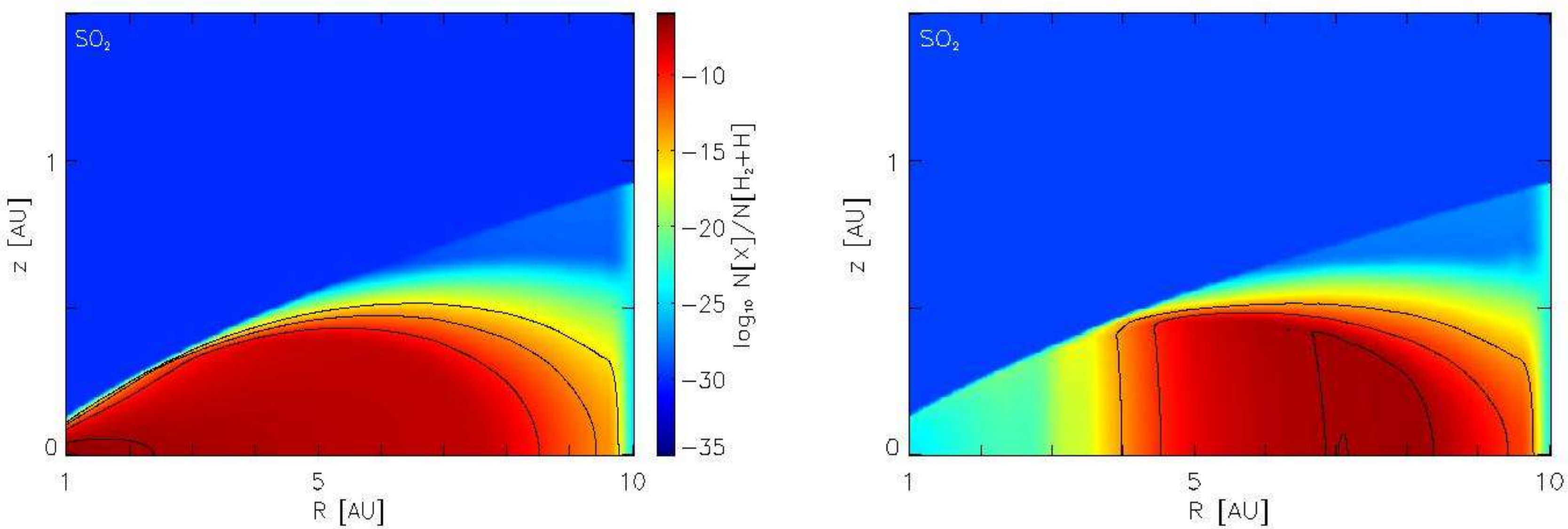
Vertical Diffusion



Radial accretion
No vertical mixing

Radial accretion
Vertical diffusion

Ilgner, Henning, Markwick, Millar, Astron. Astrophys., 415, 613 (2004)

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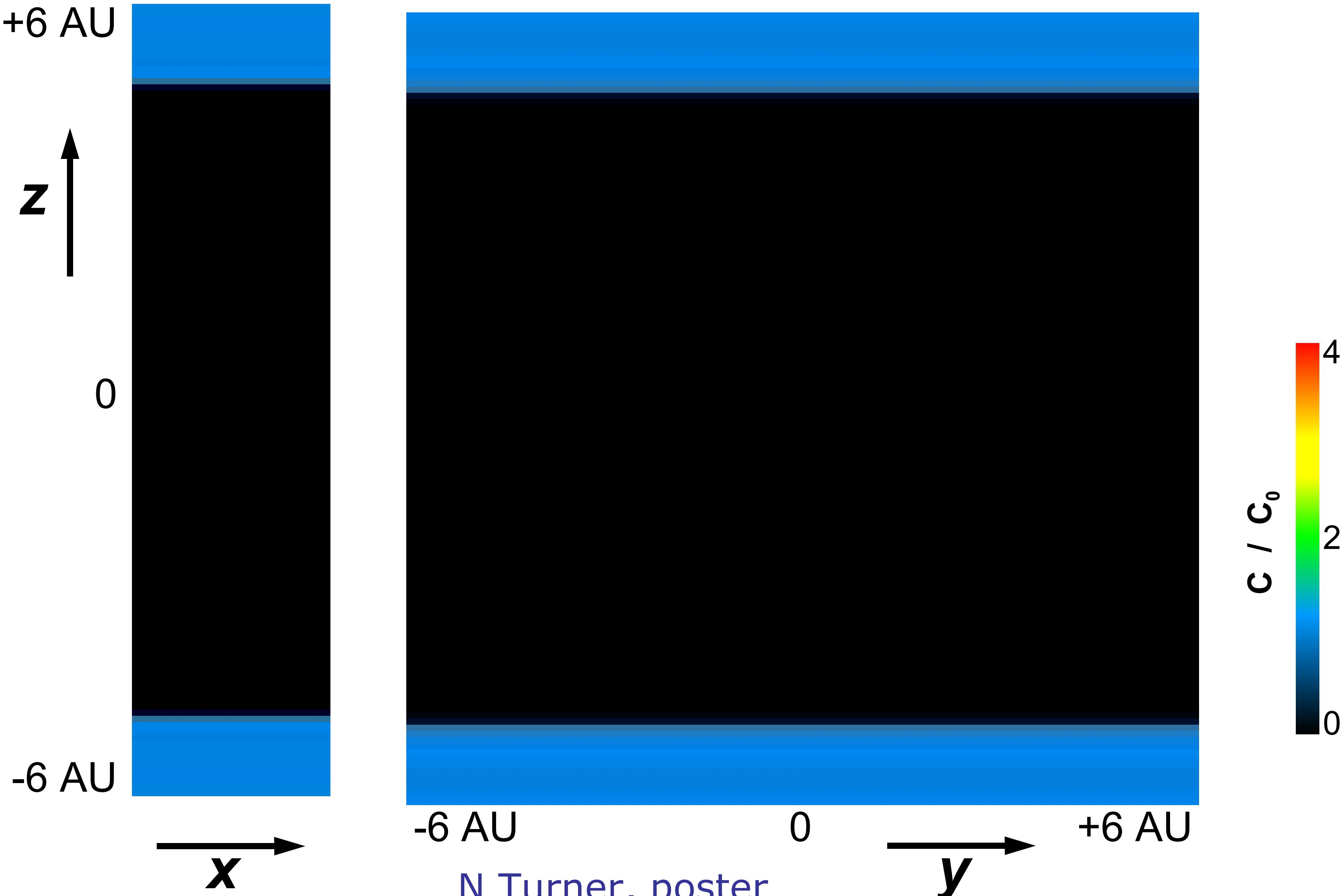
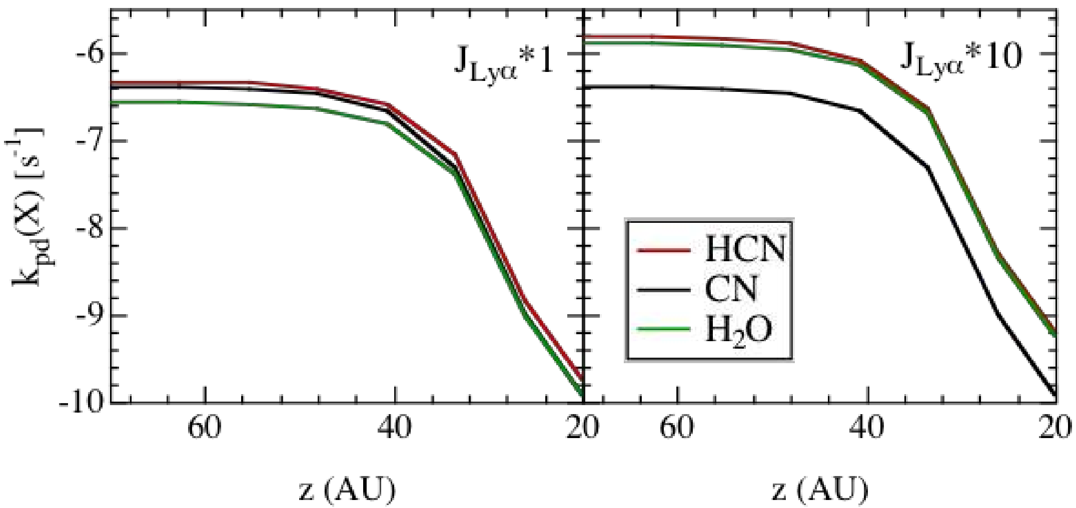
Mixing in Turbulence Driven by MRI



N Turner, poster

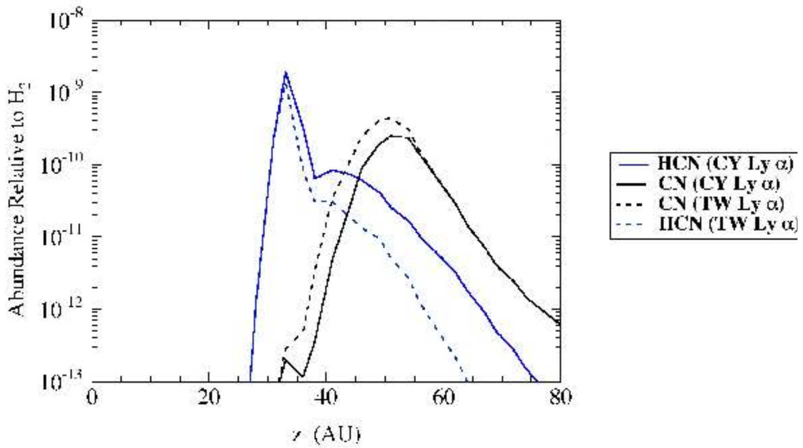
Effects of Lyman Alpha

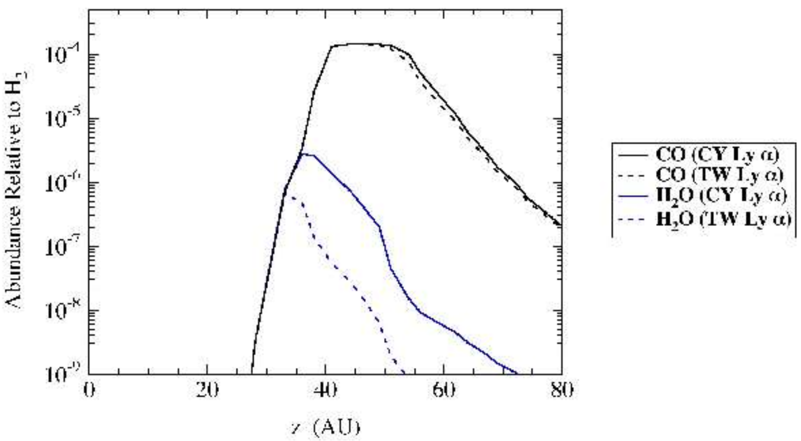


Only particular molecules have cross-sections which absorb Lyman alpha, for example HCN and H_2O but not CN and CO

E Bergin et al. ApJ, 591, L159 (2003)

Effects of Lyman Alpha

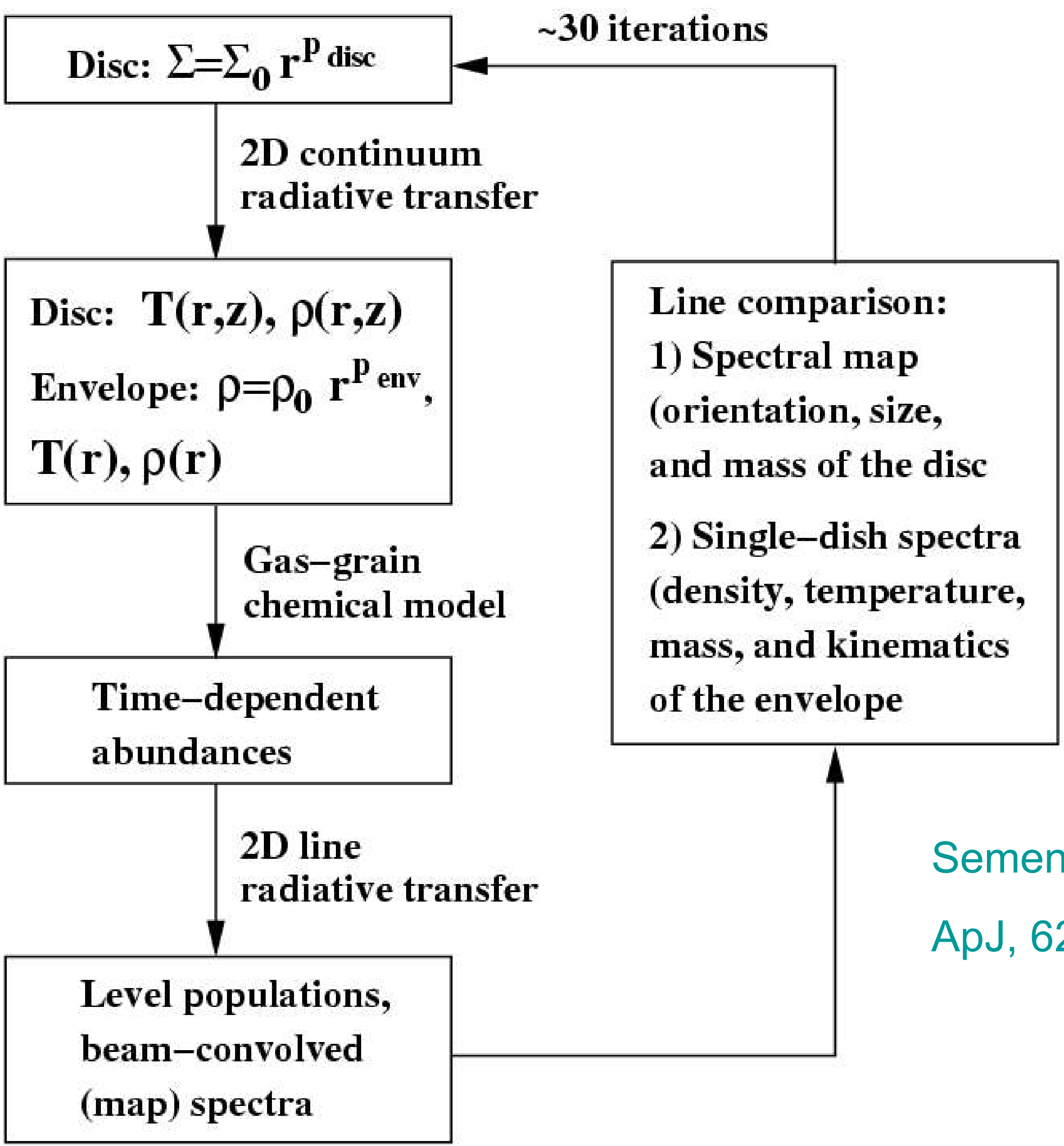




Effects of Lyman alpha on radial fractional abundances

E Bergin

Modelling scheme



Semenov et al.

ApJ, 621, 853, 2005

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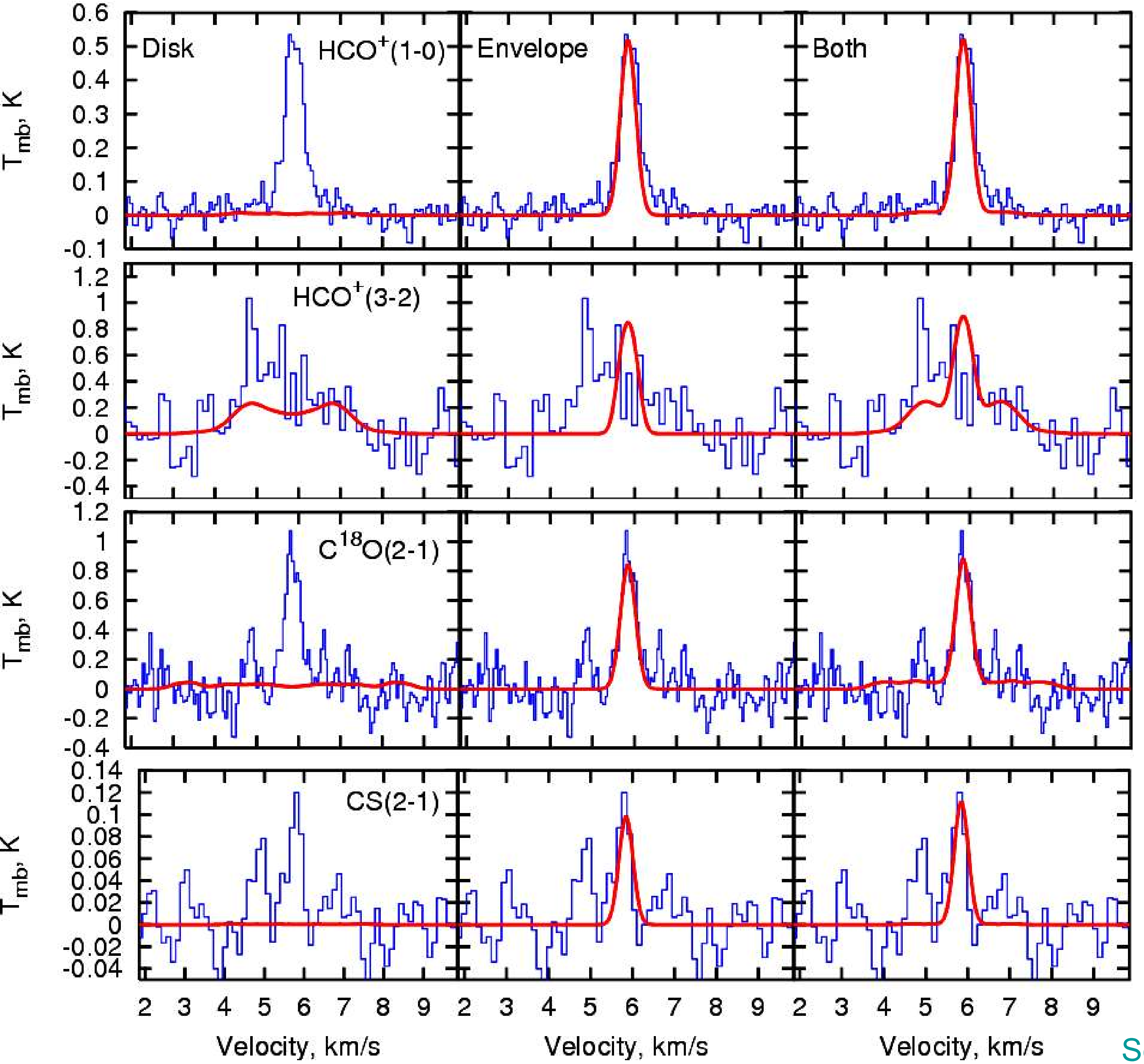
Density structure of the envelope in AB Aur



- HCO$^+$(1-0): n_0=4·10^5 cm^{-3}
- (3-2)/ (1-0): p=1±0.3
- CS(5-4): only "clumpy" model works!
- Total mass: ~1 M_{sun}
- Accretion rate: ~4·10^{-8} M_{sun} / yr
- Lifetime: <25 My

Semenov et al

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Future

From models of IS chemistry:

- Better understanding of gas-grain interaction - binding energies, surface chemistry, desorption
- Influence of PAHs on chemistry
- Key reaction rate coefficients

Model calculations:

- Ability to compare models quantitatively - same disk model but different chemistries; same chemistry but different disk models
- Better exploration of phase space

Realistic physical models

- Stellar UV including Lyman alpha
- Grain opacity including growth and sedimentation
- Diffusion, turbulence, mixing