Chemical Evolution of Protoplanetary Disks

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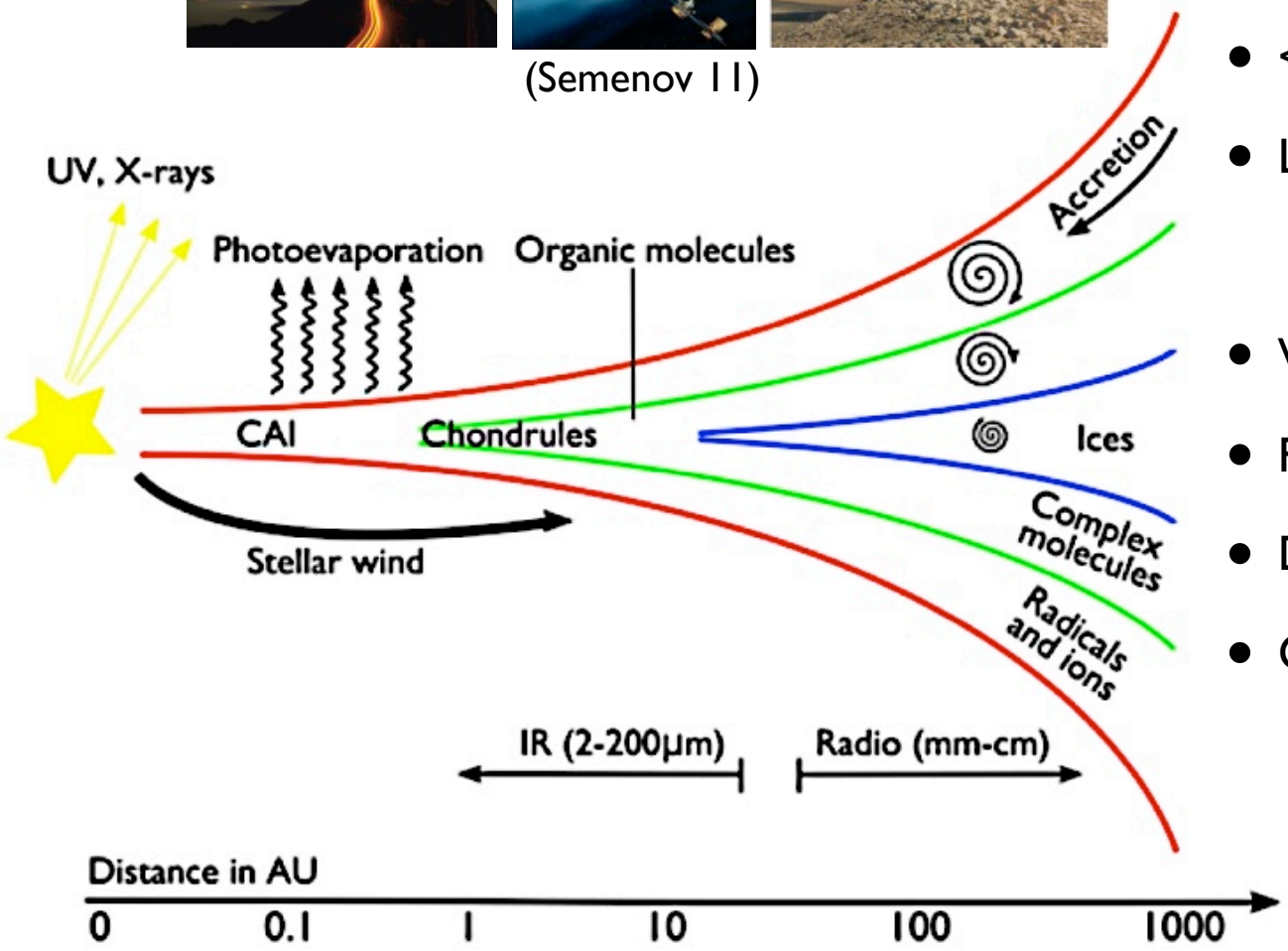
Credit: David E. Thrilling

A scheme of disk structure



(Semenov 11)



- ≲ 1% of star mass
- <50 – 1000 AU
- Lifetime: ~1 – 10 Myr

- Wide range of T & ρ
- FUV, X-rays, cosmic rays
- Dynamical evolution
- Grain evolution

Astrochemistry modeling

$$\frac{\partial n_i}{\partial t} = \sum_{j,k \neq i} k_{jk} n_j n_k - n_i \sum_l k_l n_l + \nabla D n_{\mathrm{H2}} \nabla n_i / n_{\mathrm{H2}} - \nabla U n_i$$

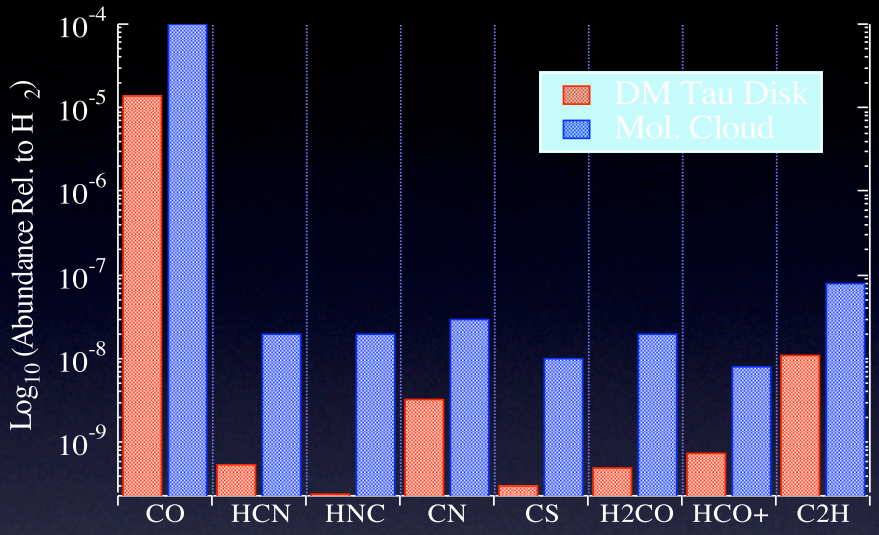
- Physical conditions
- Initial abundances of molecules
- Grain properties
- Chemical reaction data:
  - Ohio State University (OSU)
  - Manchester University (UMIST)
  - KIDA (Bordeaux)
  - ~10 – 20% rates are accurate

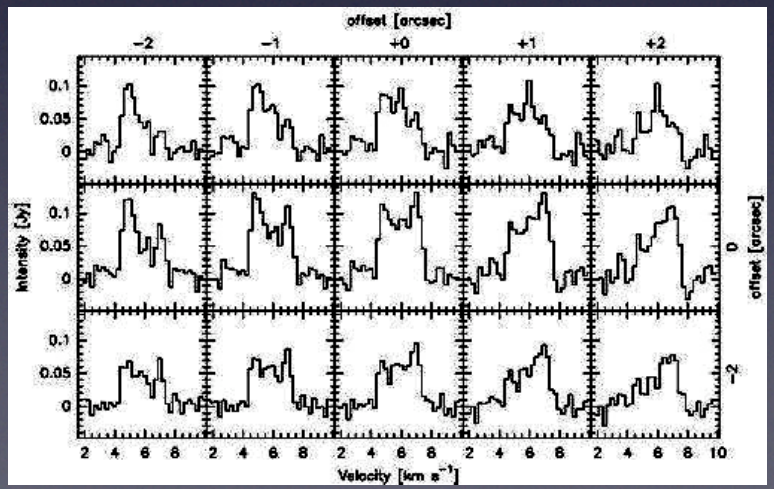
(Willacy & Langer 00; Aikawa ++02; Markwick ++02; van Zadelhoff ++03; Ilgner ++04; Kamp & Dullemond 04; Semenov ++05; Aikawa & Nomura 06; Tscharnuter & Gail 07; Agúndez ++08; Woods & Willacy 09; Walsh ++10; Semenov & Wiebe 11)

Observational findings

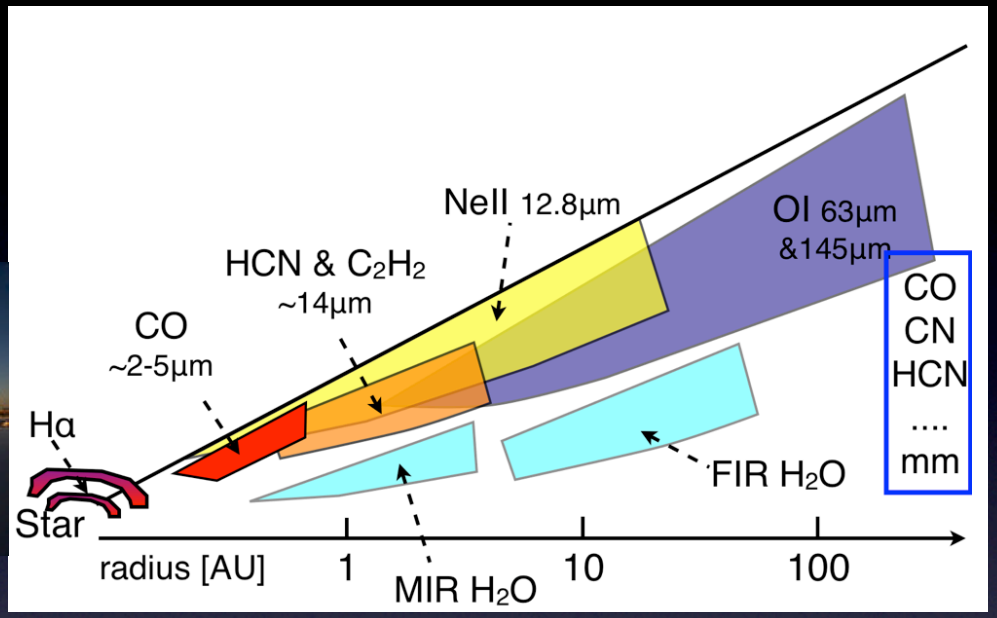
- Depletion in outer disks (x5 – 100)
- Photo-dominated chemistry
- Cold CO, CCH, HCN
- "Dry" interiors
- Isotopic fractionation
- Grain growth
- Rich composition of inner disks

(Bergin ++07; Dutrey ++07; Semenov ++10)

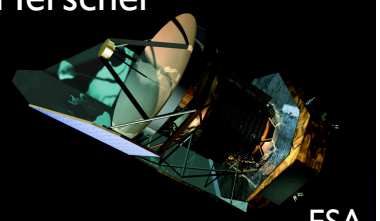




IR revolution: chemistry in planet-forming zones



Herschel



ESA

- NeII, FeII, OI, H_2, OH, H_2O, CO_2, HCN and C_2H_2
- T ≳100 – 5000 K
- No depletion
- Herbig Ae systems show less rich molecular spectra (H_2O)
- Photo- and endothermic chemistry
- Fischer-Tropsch/combustion chemistry?

(Lahuis ++ 06, Pascucci ++ 07-11, Salyk ++ 08-11, Pontoppidan ++ 07-11, Carr & Najita 08, Kamp++11)

Chemistry in T Tau and Herbig Ae outer disks

- "Chemistry in Disks" (PdBI): >6 disks
- Observations + modeling
- DISCS (SMA): 12 disks
- Herbig Ae: CO, HCO^+, CN, HCN
- T Tau: CO, HCO^+, HCN, N_2H^+, CCH, CS, H_2CO, DCO^+, DCN

- Surface densities and T_{kin} are OK
- HAe disks are molecularly poor?

- Low $L_{X\text{-}ray}$ in HAe: No CO + $He^+ \rightarrow C^+ + O + He$
- No low-T surface chemistry in HAe disks

(Dutrey ++ 07; Schreyer ++ 08; Henning ++ 10; Öberg ++ 10-11)

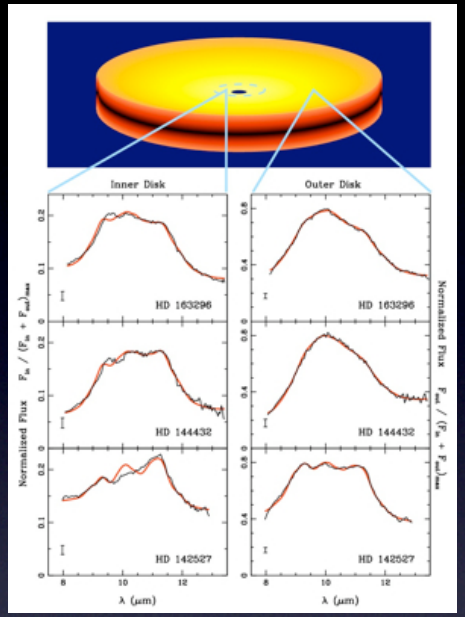
Chemistry with dynamics

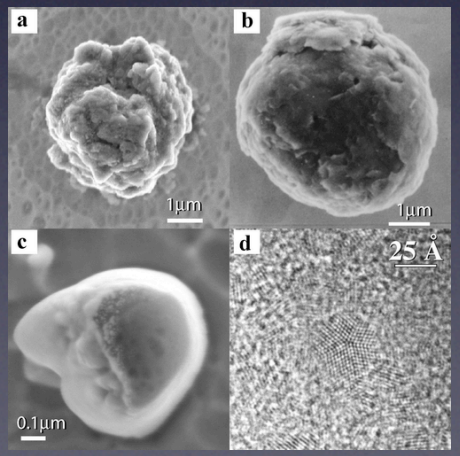
- Turbulence & accretion
- Isotopic homogeneity of the Solar Nebula
- Crystalline silicates in comets and outer disk regions

- Extended gas-grain chemistry
- 1D/2D turbulent mixing
- "ALCHEMIC" code

- "Qualification" fit to observations
- Reduced and oxidized ices in comets

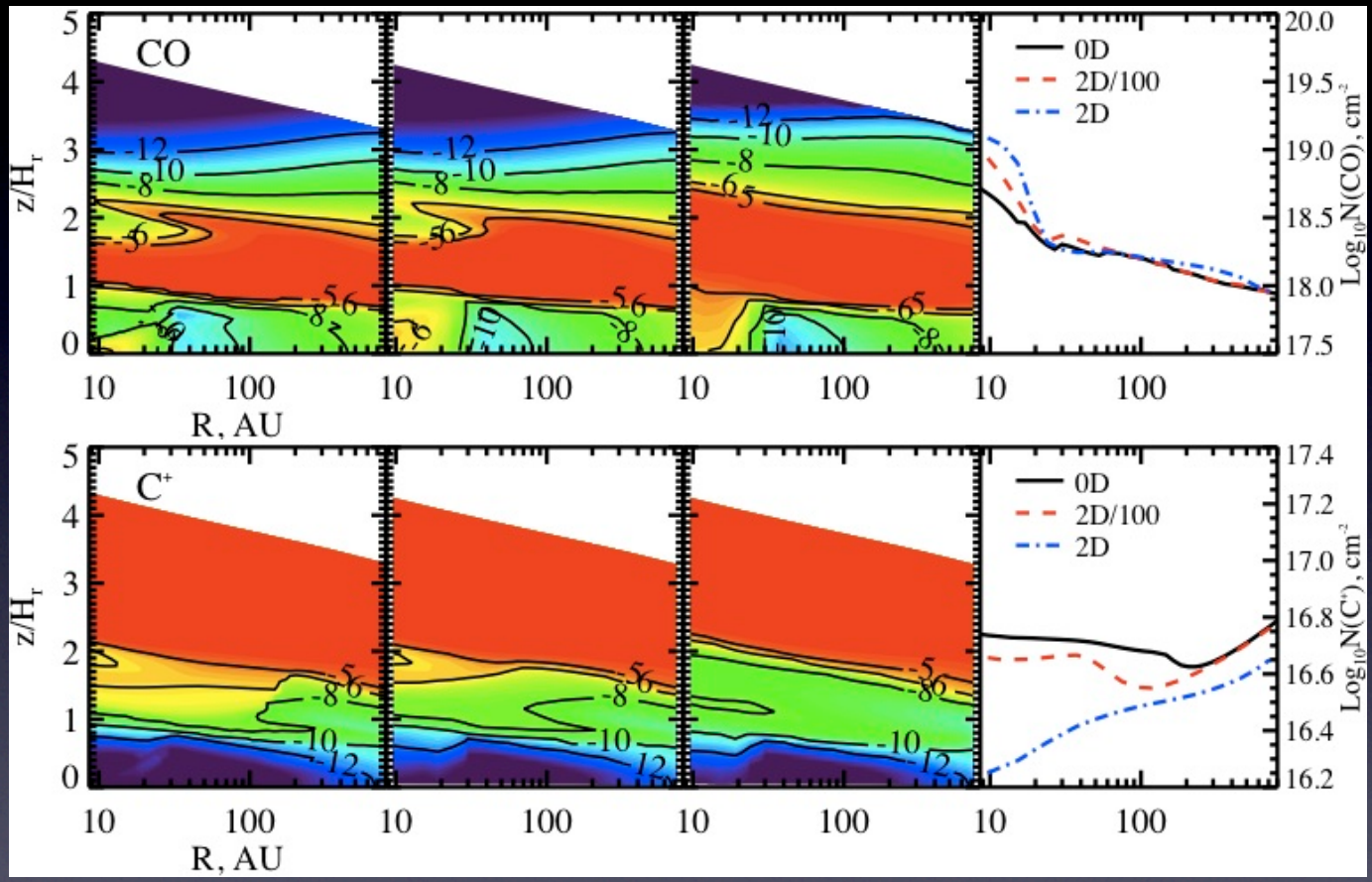
(Ilgner ++04, Willacy ++06; Nomura ++09; Hersant ++ 10;
Heinzeller ++11; Semenov ++10; Semenov & Wiebe 11)





Steadfast species

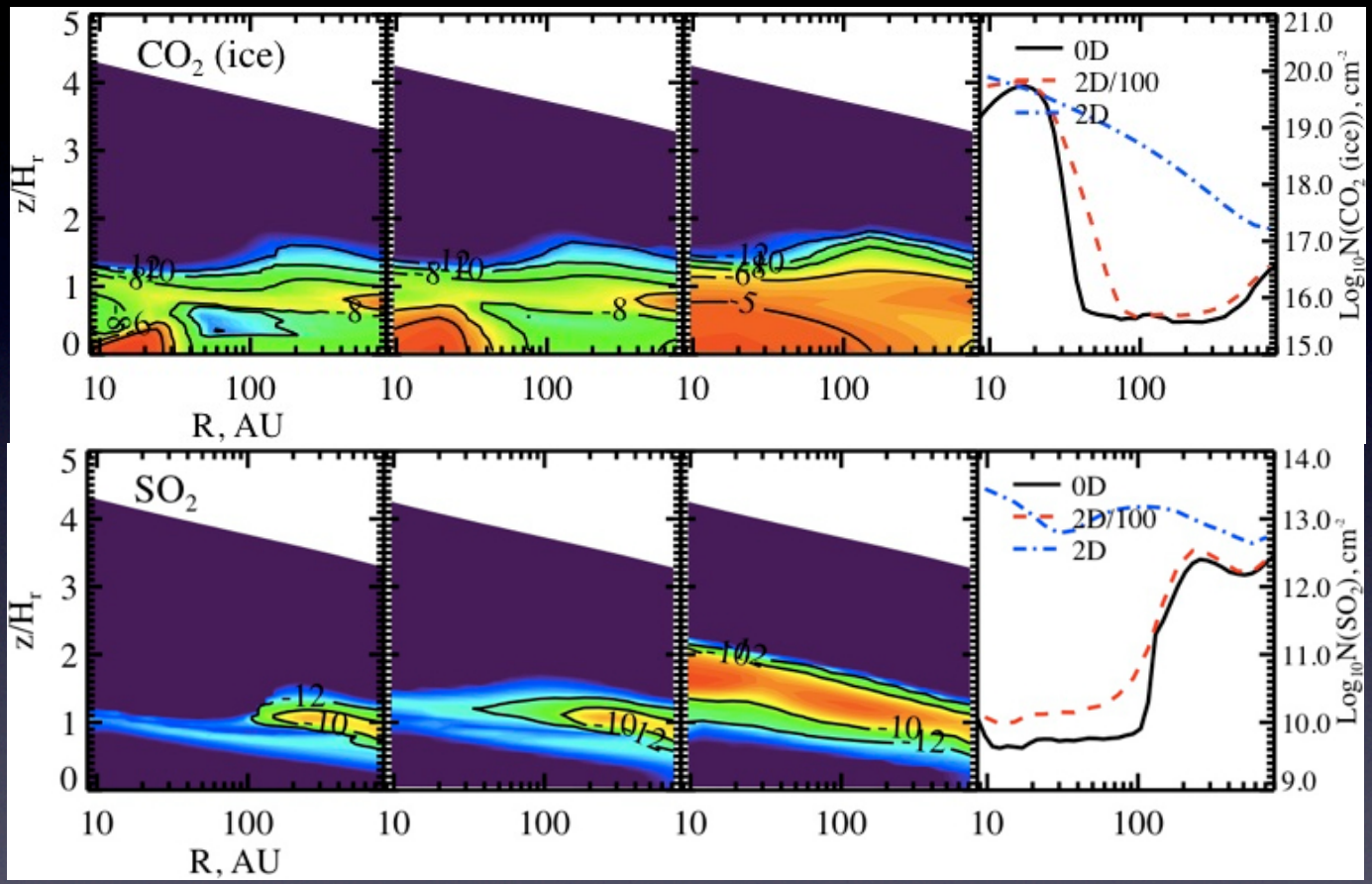
Laminar Slow Mixing Fast Mixing Column Densities



- Fast gas-phase formation and destruction
- Gas-phase chemistry < Dynamics
- Example: CO, OH, H_2O ice, CCH, C^+, CN, HCN

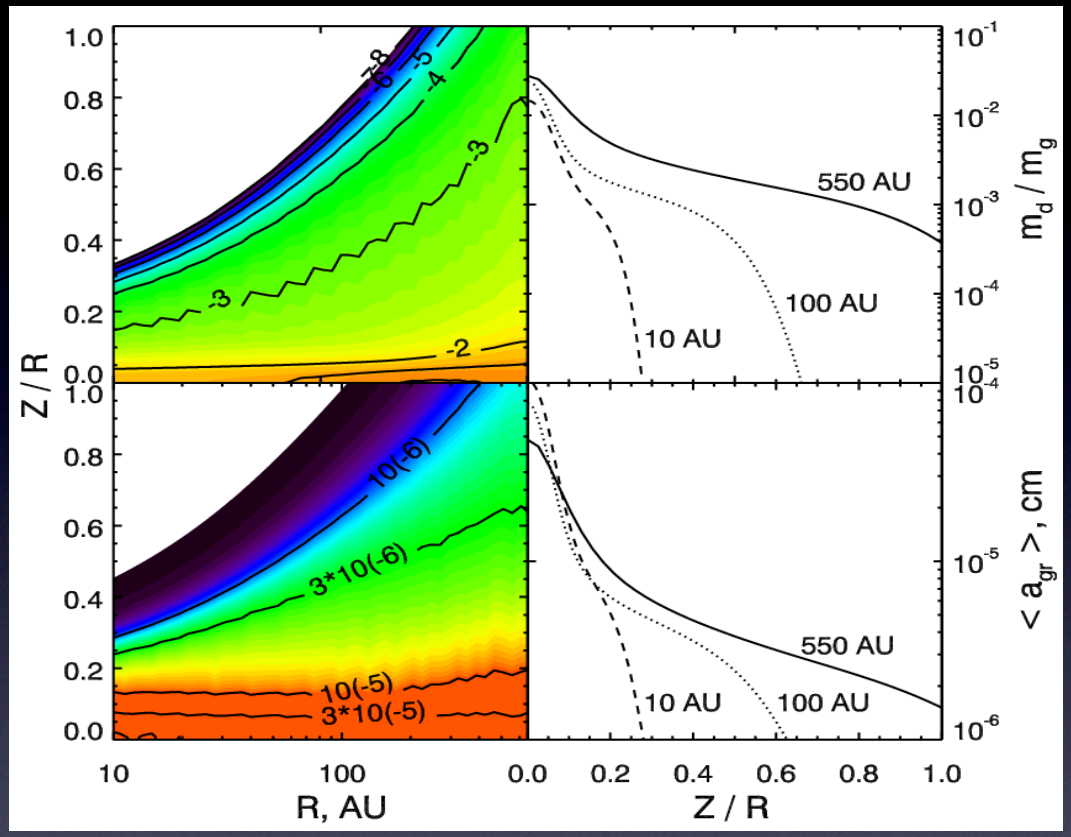
Sensitive species

Laminar Slow Mixing Fast Mixing Column Densities



- (Partly) slow surface formation, slow desorption
- Surface chemistry > Dynamics
- Hydrocarbons (e.g., C_2H_2), organics (HCOOH), SO, SO_2, C_2S, C_3S

Chemistry with grain growth

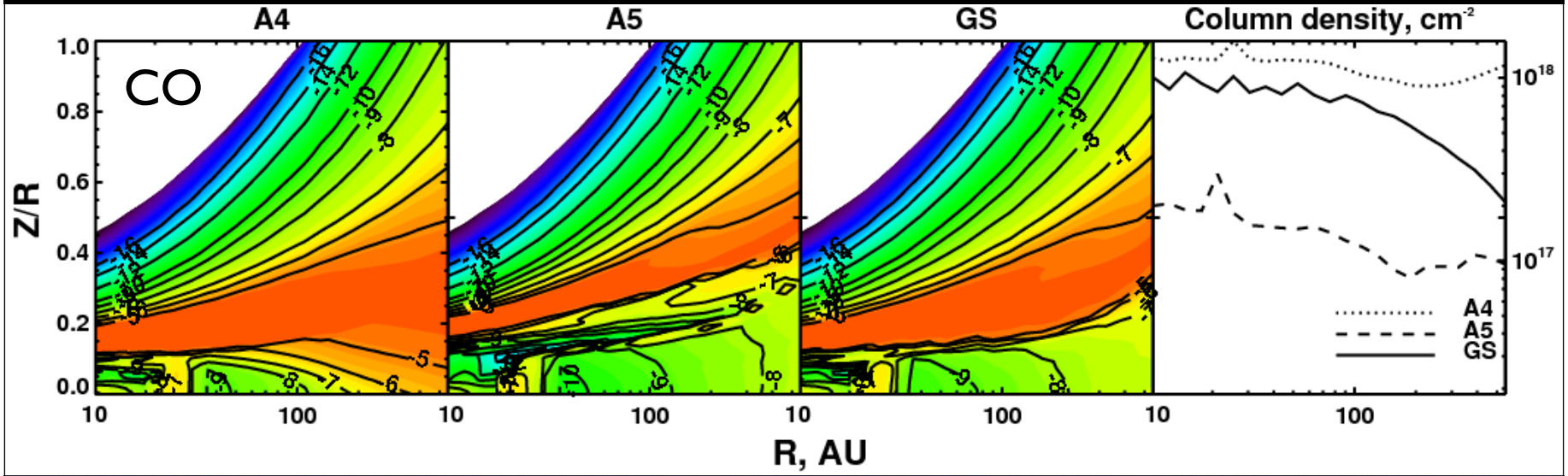


- Small grains stays up, big grains settle down
- <Grain size> decreases outward
- FUV reach deepr disk regions

(Aikawa & Nomura 06, Fogel ++11, Vasyunin ++11)

Chemistry with grain growth

Uniform dust, 1 μm Uniform dust, 0.1 μm Evol. model Column Densities

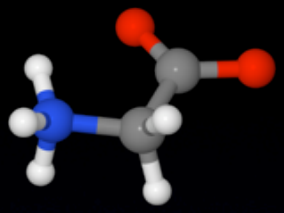


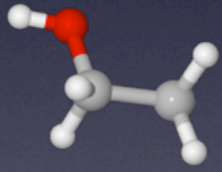
- Molecular layers shift down & expand
- Depletion zone shrinks
- Tracers of grain growth: e.g., C_2H_2/HCN, CO, CN, and SO
- Tracers of Ly_a: e.g., HCN, NH_3, and CH_4
- Better "qualification" agreement with observations

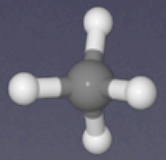
Conclusions

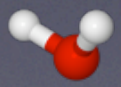
- Inner disk region
- High-energy radiation
- Dynamical processes
- Grain evolution

- Basic disk chemistry is understood
- "Cool" vs "warm" disks
- Large observational & modeling programs
- Crude chemo-dynamical models



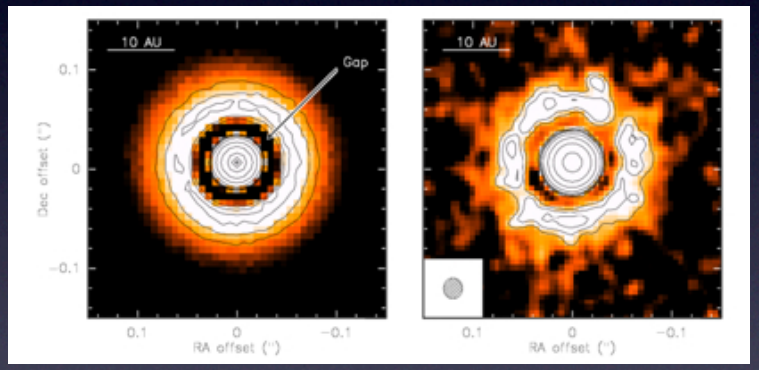


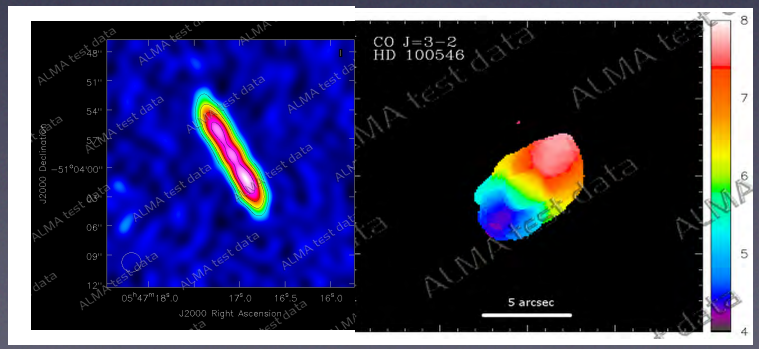




ALMA: The Brave New World

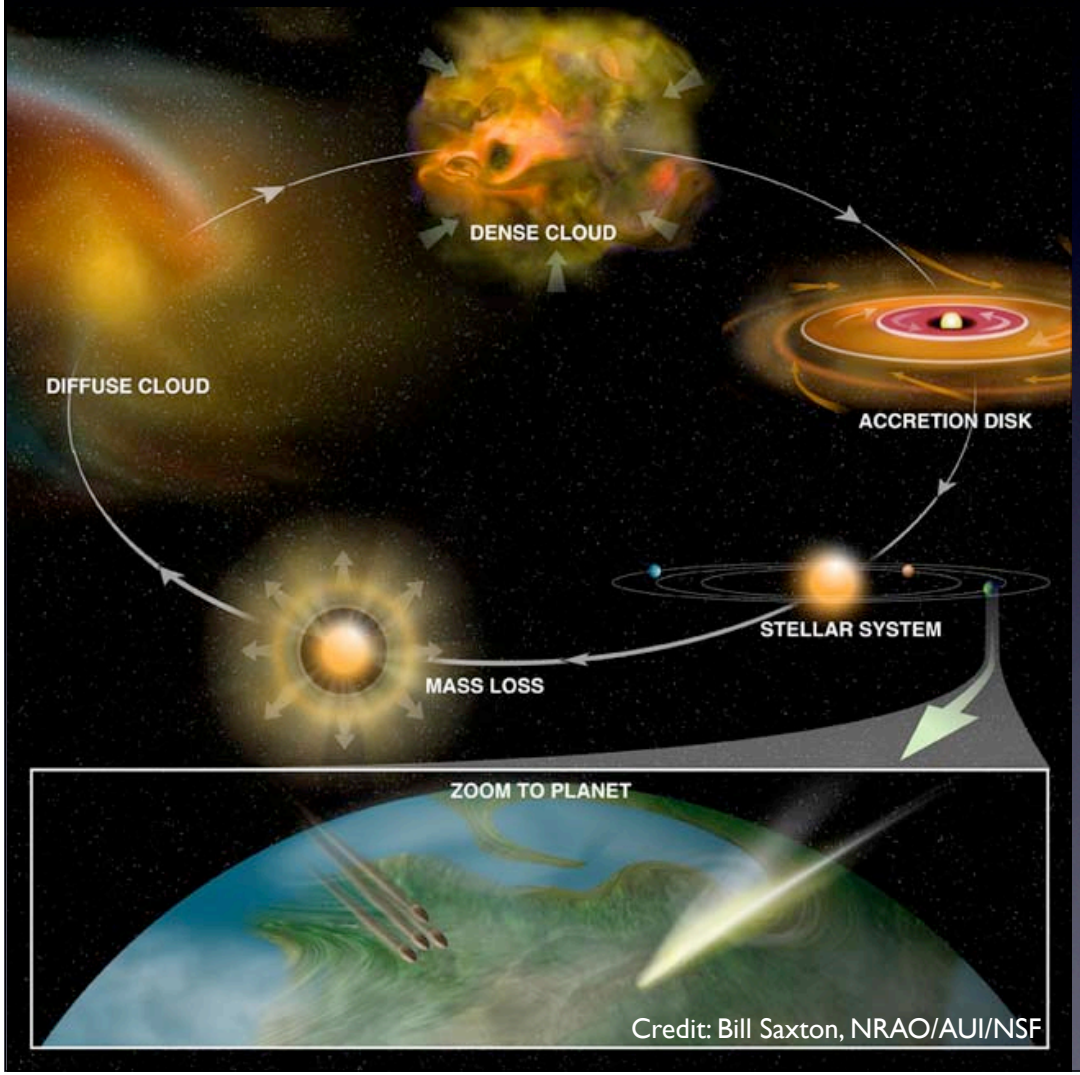
- Atacama Large Millimeter Array (2013)
- 50 x 12m + 12x7m + 4x12m
- High resolution (0.005″), <0.05 km/s
- 86 – 950 GHz (250 μm – 1 mm)





- Complex molecules: organics, hydrocarbons, N, S, P, ...-bearing
- Isotopologues: ^{15}N, ^{34}S, ^{17,18}O, D
- Planet-formation regions
- Molecular layers
- Large- and small-scale dynamics
- Large surveys
- Unknown unknowns!

Disks are birth sites of planetary systems



- Initial stages of planet formation
- Primordial atmospheres
- Primitive bodies
- Genesis of organic molecules

- Molecules are probes:
- Physical conditions
- Kinematics
- Chemical complexity