Disk Chemistry

T. J. Millar,

School of Physics and Astronomy, University of Manchester
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)

\[ n(\text{H}_2) \sim 10^{10} - 10^{15} \text{ cm}^{-3} \]

Molecular gas is frozen on to dust grains in outer disk

Temperature of inner disk is \( \sim 100 \text{ K at 10 AU, } \sim 1000 \text{ K at 1 AU} \)

Ices evaporate in inner disk
Chemical Processes

Ionization – X-rays, UV photons (direct + scattered + 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

$\text{H}_2$ self-shielding, $\text{C}^+/\text{C}/\text{CO}$ transition

UV excess ? Lyman alpha ?

Grain opacity

composition, size distribution

Gas cooling – O, $\text{C}^+$, C, CO

Dust heating/cooling – photoelectric emission

gas-grain collisions

Time-dependent or steady-state chemistry ?

Stellar heating ?
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 ?
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\textsubscript{2} reactions – very sensitive to high T regime
Vertical temperature distribution

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

Heating causes expansion of disk vertically.

Dust and gas temperatures decouple.

Density distribution
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

Molecular Distributions

Disk ionization degree at 1 Myr

Gas-grain chemistry,
$t = 10^6$ yrs

Surface (UV, X-rays)
Intermediate (X-rays)
Midplane (CR, RN)

Semenov, Wiebe, Henning
Chemical differentiation in z-direction

Surface layer (hot):
PDR-like chemistry (X-rays and UV),
H$^+$, He$^+$, C$^+$, CN, C$_2$H

Intermediate layer (warm):
Rich molecular chemistry (X-rays), surface reactions, desorption,
CS, CO, NH$_3$, H$_2$CO, HCO$^+$, HCNH$^+$, NH$_4^+$, H$_3$CO$^+$, S$^+$, He$^+$

Midplane (cold):
Dark chemistry (CR and RN), ‘total’ freeze out,
Metal ions, H$_3^+$, HCO$^+$, N$_2$H$^+$, H$_2$D$^+$, D$_2$H$^+$, D$_3^+$
Cold, depleted gas drives multiple deuteration

\[ \text{H}_3^+, \text{H}_2, \text{H} \quad \text{e}^- \quad \text{HD}, \text{H}_2, \text{D}, \text{H} \quad \text{HD}, \text{D}_2, \text{D}, \text{H} \quad \text{D}_2, \text{D} \]

\[ \text{HCO}^+, \text{N}_2\text{H}^+, \text{OH}^+ \quad \text{DCO}^+, \text{HCO}^+, \text{N}_2\text{D}^+, \text{N}_2\text{H}^+, \text{OD}^+, \text{OH}^+ \quad \text{DCO}^+, \text{N}_2\text{D}^+, \text{OD}^+ \]

(See poster by Dominik)
Vertical Diffusion

Radial accretion
No vertical mixing

Radial accretion
Vertical diffusion

Mixing in Turbulence Driven by MRI

N Turner, poster
Only particular molecules have cross-sections which absorb Lyman alpha, for example HCN and H$_2$O but not CN and CO

Effects of Lyman Alpha

Effects of Lyman alpha on radial fractional abundances

E Bergin
Modelling scheme

Disc: $\Sigma = \Sigma_0 r^p_{\text{disc}}$

2D continuum radiative transfer

Disc: $T(r,z), \rho(r,z)$
Envelope: $\rho = \rho_0 r^p_{\text{env}}, T(r), \rho(r)$

Gas–grain chemical model

Time–dependent abundances

2D line radiative transfer

Level populations, beam–convolved (map) spectra

~30 iterations

Line comparison:
1) Spectral map (orientation, size, and mass of the disc)
2) Single–dish spectra (density, temperature, mass, and kinematics of the envelope)

Semenov et al.
Density structure of the envelope in AB Aur

- **HCO$^+$ (1-0):** $n_0 = 4 \cdot 10^5$ cm$^{-3}$
- **(3-2)/(1-0):** $p = 1 \pm 0.3$
- **CS (5-4):** only "clumpy" model works!
- **Total mass:** $\sim 1 M_{\text{sun}}$
- **Accretion rate:** $\sim 4 \cdot 10^{-8} M_{\text{sun}} / \text{yr}$
- **Lifetime:** $< 25 \text{ Myr}$

Semenov et al
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