Modelling of protoplanetary disks

A “cookbook” for observationally-motivated disk physico-chemical models

Catherine Walsh
NWO Veni Fellow
Leiden Observatory
Observations of protoplanetary disks

Until recently: only spatially-unresolved observations were possible (with single-dish telescopes)

Dust

Dust spectral energy distribution

Gas

Molecular/atomic emission lines

\(^{12}\)CO \(J = 3-2\)

\(i \sim 0^\circ\) \hspace{1cm} \(i \sim 40^\circ\)

General outline of a physico-chemical model

- Laboratory data
- Chemical model
- Physical model
- Astrophysical observations
- Chemical abundances
- Molecular line radiative transfer
- Continuum radiative transfer
- Simulated observations

Comparing and contrasting
Outline

Disk physical structure:
- dust
- gas

Disk chemical structure:
- gas-phase (vapour)
- solid-phase (ice)

Building physico-chemical models
Observations of dust in protoplanetary disks

Early modelling efforts concerning the dust focussed primarily on reproducing the spectral energy distribution (SED)

- Optical wavelengths: scattered light; hence no temperature/density information
- Near-infrared wavelengths: originates mainly from “hot” inner rim
- Mid-infrared wavelengths: originates from “warm” dust close to the star (< 10 AU) and is typically optically thick; hence, no density information but probes temperature of dust photosphere
- Sub-mm/mm wavelengths: originates from “cold” dust in outer disk (> 10 AU) and is typically optically thin; hence, has both temperature and density information
Observations of dust in protoplanetary disks

Observations of dust in protoplanetary disks

Some simple assumptions about the (sub)mm opacity and dust temperature can yield an estimation of the disk mass.

Dust spectral energy distribution

Optical depth

\[ \tau_v = \int \rho \kappa_v ds = \kappa_v \Sigma, \]

Dust mass opacity

\[ \kappa_v = 0.1 \left( \frac{\nu}{10^{12} \text{Hz}} \right)^\beta \text{cm}^2 \text{g}^{-1}. \]

Disk mass

\[ M_{\text{gas + dust}} = \frac{F_v d^2}{\kappa_v B_v(T)}, \]

Gas-to-dust mass ratio \( \sim 100 \)

Observations of dust in protoplanetary disks

The advent of (sub)mm interferometry required more sophisticated models to describe the radial disk structure.

Disk surface density, temperature, and dust mass opacity were “well-fit” using power laws:

\[
T_r = T_1 \left( \frac{r}{1 \text{ AU}} \right)^{-q},
\]

\[
\Sigma_r = \Sigma_5 \left( \frac{r}{5 \text{ AU}} \right)^{-p},
\]

\[
\kappa_\nu = \kappa_0 \left( \frac{\nu}{\nu_0} \right)^\beta,
\]

Observations of dust in protoplanetary disks

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\[ F_\nu = \frac{\cos i}{d^2} \int_{r_0}^{R_d} B_\nu(T_r)(1 - e^{-\tau_\nu,r \sec i})2\pi r \, dr, \]

\[ \Sigma_r = \Sigma_5 \left( \frac{r}{5 \text{ AU}} \right)^{-p}, \]

\[ \kappa_\nu = \kappa_0 \left( \frac{\nu}{\nu_0} \right)^{\beta}, \]
Observations of dust in protoplanetary disks

Fitting is done directly to the interferometric data (so-called visibilities) which are the Fourier transform of the intensity distribution.
Observations of dust in protoplanetary disks

Higher-resolution (sub-arcsecond) interferometric data required additional considerations for models of the dust emission: cavities and rings

SMA observations
Evolution of dust in protoplanetary disks

Generalised picture of dust evolution in protoplanetary disks

Small grains are well coupled to the gas

Large grains formed by coagulation settle towards the midplane

Large grains drift inwards due to headwind from gas

Cavities form due to planets/photoevaporation

Eventually dust is incorporated into larger bodies or expelled in photoevaporative flow

Small (~ μm-sized) and large (~ mm-sized) grains follow different paths

Simple power-law models are still used, but with gaps and cavities, and “small” and “large” grains are decoupled to simulate settling. Despite more complex models being used to model more complex data, significant degeneracies still remain in the models.
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Modelling of dust in protoplanetary disks

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\[ \Sigma_g = \Sigma_c \left( \frac{R}{R_c} \right)^{-\gamma} \exp \left[ -\left( \frac{R}{R_c} \right)^{2-\gamma} \right], \]

\[ \rho_s = \frac{(1-f)\Sigma}{\sqrt{2\pi Rh}} \exp \left[ -\frac{1}{2} \left( \frac{\pi/2-\Theta}{h} \right)^2 \right], \]
Dust opacity

The dust density and size distribution sets the temperature structure of the disk: dust composition and opacity are required.

Single MRN size distribution: \( \frac{dn}{da} = C \times a^{-3.5} \)

Two-populations of MRN-like grains: “small” and “large”
How do we know the composition of the dust?

The dust emission at mid- to far-IR wavelengths shows spectral features which can be attributed to different grain components.
How do we know disks are flared?

Spatially-resolved mid-IR imaging has revealed the flared morphology of emission from small grains (PAHs) in nearby protoplanetary disks.

VISIR @ 8.6 μm
ALMA @ 1 mm

Dust
CO

Disk emission is “flat” at (sub)mm wavelengths: evidence for settling

HD 97048: a group I Herbig Ae disk

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Dusty disks in the era of ALMA

Highly asymmetric (sub)mm dust emission attributed to dust trapping in vortices potentially created by forming planets

Are these the exception rather than the norm? Both are A-type stars

Dusty disks in the era of ALMA

Highly symmetric and concentric rings attributed to various mechanisms, including dust traps, sintering, condensation fronts, ...
Dusty disks in the era of ALMA

Highly symmetric and concentric rings attributed to various mechanisms, including dust traps, sintering, condensation fronts, ...

HL Tau

TW Hya
Dusty disks in the era of ALMA

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HL Tau  
TW Hya
What about the gas?

Gas is mainly $\text{H}_2$ (90%) and He (10%) which are difficult to observe: CO (~0.01%) is used as a proxy as the second-most abundant molecule.

Warning! CO gas can have a complex distribution due to the disk structure.
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Warning! CO gas can have a complex distribution due to the disk structure.
What about the gas?

Emission from the main CO isotopologues (\(^{12}\)CO and \(^{13}\)CO) are optically thick, hence less abundant isotopologues are used (\(C^{18}O\) and \(C^{17}O\))

**Dust and gas masses from the ALMA Survey of Lupus**

Increasing dust mass

No clear trend

Gas-to-dust mass ratios from ~ 1000 - 10
What about the gas?

Emission from the main CO isotopologues ($^{12}$CO and $^{13}$CO) are optically thick, hence less abundant isotopologues are used ($^{18}$O and $^{17}$O).

![Graph showing dust and gas masses from the ALMA Survey of Lupus](image)

Dust and gas masses from the ALMA Survey of Lupus

What about the gas?

Picture is further complicated by chemical effects, namely, isotope-selective photodissociation

\[
\begin{align*}
\frac{^{12}\text{C}}{^{13}\text{C}} & \sim 77 \\
\frac{^{16}\text{O}}{^{18}\text{O}} & \sim 560 \\
\frac{^{16}\text{O}}{^{17}\text{O}} & \sim 1792
\end{align*}
\]
What about the gas?

Given the relative complexity of interpreting CO observations, HD (~0.001% of H$_2$) is proposed as an alternative tracer of the gas mass.

Disk mass (TW Hya) > 0.05 M$_{\text{sol}}$

CO line emission in the ALMA era

ALMA Cycle 0 observations of CO $J=3-2$ emission from HD 163296

CO J=3-2 shows emission from a moderately flared disk (z/r ~ 0.1) and reveals evidence of CO freezeout in the disk midplane.
CO line emission in the ALMA era

ALMA Cycle 0 observations of CO J=3-2 emission from HD 97048

CO emitting layer is very flared: z/r ~ 0.7-1.0

Modelling the gas and dust in tandem

Gas surface density still assumed to follow the dust: gas-to-dust mass ratio is now a “free” (yet still global) parameter.

Towards a global prescription of gas and dust

Modern models now fit the dust SED and spectrally and spatially resolved molecular line observations simultaneously.
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TW Hya: a T Tauri disk
Observations of protoplanetary disks

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Dust spectral energy distribution

Molecules/atomic emission lines

\(^{12}\text{CO} \ J =3-2\)

Dust

Gas

Ices

Molecules

Atoms and ions

Observations of protoplanetary disks

Until recently: only spatially-unresolved observations were possible (with single-dish telescopes)

What about the chemistry? So far H$_2$, HD, and CO only mentioned! Useful probes of disk structure only.

Dust spectral energy distribution

Molecules

Atoms and ions

Molecular/atomic emission lines

$^{12}$CO J = 3-2
The astronomers’ periodic table

http://www.chandra.harvard.edu
The astronomers’ periodic table

Main components of abundant molecules/volatiles (ice and gas)

http://www.chandra.harvard.edu
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- ✴ Cations (positively-charged)
- ✴ Anions (negatively-charged)
- ✴ Radicals (unpaired electrons)
- ✴ Unsaturated carbon chains
- ✴ Structural isomers
- ✴ Complex organic molecules
- ✴ Many isotopologues
- ✴ > 180 and counting ...

http://www.astro.uni-koeln.de/cdms/molecules
# Molecules in space

## Table of Molecules

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[http://www.astro.uni-koeln.de/cdms/molecules](http://www.astro.uni-koeln.de/cdms/molecules)
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<td>HCS⁻</td>
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</tbody>
</table>

Protoplanetary disk molecules/volatiles?

21* and counting …

* not including isotopologues

http://www.astro.uni-koeln.de/cdms/molecules
Detection of molecules

A crash course in molecular spectroscopy

Detection of molecules

A crash course in molecular spectroscopy

E = \( E_{rot} + E_{vib} + E_{el} \)

Increasing energy
Detection of molecules

A crash course in molecular spectroscopy

\[ E = E_{rot} + E_{vib} + E_{el} \]

Ground electronic state

Excited electronic state

Rotational emission at (sub)millimeter to centimeter wavelengths

Vibrational absorption/emission at infrared wavelengths

Electronic absorption at ultraviolet to visible wavelengths

Increasing energy

10–100 K
Detection of molecules

A crash course in molecular spectroscopy

$E = E_{rot} + E_{vib} + E_{el}$

Increasing energy

100–1000 K

Rotational emission at (sub)millimeter to centimeter wavelengths

Vibrational absorption/emission at infrared wavelengths

Ground electronic state

Excited electronic state

Electronic absorption at ultraviolet to visible wavelengths

$J = 0$

$J = 1$

$J = 2$

$v = 0$

$v = 1$
Detection of molecules

Rotational transitions: $\text{H}_2\text{O}$

$I_A \neq I_B \neq I_C$

Despite only consisting of 3 atoms, $\text{H}_2\text{O}$ has a complex rotational spectrum

Detection of molecules

Vibrational transitions: H₂O
Detection of molecules

Vibrational transitions: $\text{H}_2\text{O}$
Detection of molecules

Infrared wavelengths: absorption

Warm to hot dust and gas

Cold gas and cold icy dust

Embedded Outflow in HH 46/47

Spitzer Space Telescope • IRS • IRAC

NASA / JPL-Caltech / A. Noriega-Crespo (SSC/Caltech)

ssc2003-06g
Detection of molecules

(Sub)millimeter wavelengths: emission

HIFI Spectrum of Water and Organics in the Orion Nebula

© ESA, HEXOS and the HIFI consortium
E. Bergin
Chemical anatomy of a protoplanetary disk

Two phases of molecules/volatiles in protoplanetary disks: gas (H$_2$ dominated) and ice (H$_2$O dominated)

Observations probe mainly the disk atmosphere: important for disk characterisation ($T,n,F_{UV},F_{XR}$, ...)

- **NEAR-IR** (1000’s K)
  - Gas (H$_2$ dominated)
    - CO, HCN, H$_2$O, OH, C$_2$H$_2$

- **MID-IR** (100’s K)
  - Gas (H$_2$ dominated)
    - CO, HCN, H$_2$O, OH, C$_2$H$_2$
  - Ices
    - H$_2$O, OH, CH$^+$, CO, HCN, HNC, SO, H$_2$CO, HC$_3$N, C$_3$H$_2$, CN, CS, C$_2$H, HCO$^+$, N$_2$H$^+$, NH$_3$, CH$_3$CN, CH$_3$OH

- **SURFACE**

- **FROZEN MIDPLANE**

- **MOLECULAR LAYER**

Stellar wind

UV
X-ray

Pontoppidan+, Gibb+, Salyk+, van Dishoeck+, Dutrey+, Chapillon+, Qi+, Oberg+, Kastner+, Thi+, Carr+, Najita+, Hogerheijde+, Fedele+, Meeus+
What chemistry is important where and why?

Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs).

Ion-molecule chemistry

Photoionisation

Photodissociation

Neutral-neutral chemistry

Gas composition

Gas cooling

T increasing

T decreasing

H₂O

H₂O

CO

CO

H₂

H₂

C⁺

C⁺

H⁺

H⁺

Hot ≥ 100 K

Cold ≤ 100 K

Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs).

What chemistry is important where and why?

Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs)

Gas composition

Ice composition

Ionisation fraction

Photoionisation

X-ray ionisation

Cosmic-ray ionisation

Formation and destruction of molecules

Gas-phase chemistry

**Bond formation**

\[ X^+ + Y \rightarrow XY^+ + \gamma_{UV} \]
\[ X^- + Y \rightarrow XY + e^- \]
\[ X + Y + M \rightarrow XY + M \]

**Bond destruction**

\[ XY + \gamma_{UV} \rightarrow X + Y \]
\[ XY + \gamma_{XR} \rightarrow X + Y \]
\[ XY + \gamma_{CR} \rightarrow X + Y \]
\[ XY^+ + e^- \rightarrow X + Y \]
\[ XY + M \rightarrow X + Y + M \]

**Bond rearrangement**

\[ X^+ + YZ \rightarrow XY^+ + Z \]
\[ X^+ + YZ \rightarrow X + YZ^+ \]
\[ X + YZ \rightarrow X + YZ \]

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021
Formation and destruction of molecules

**Gas-phase chemistry**

**Bond formation**

\[ X^+ + Y \rightarrow XY^+ + \gamma_{UV} \]
\[ X^- + Y \rightarrow XY + e^- \]
\[ X + Y + M \rightarrow XY + M \]

**Bond destruction**

\[ XY + \gamma_{UV} \rightarrow X + Y \]
\[ XY + \gamma_{XR} \rightarrow X + Y \]
\[ XY + \gamma_{CR} \rightarrow X + Y \]
\[ XY^+ + e^- \rightarrow X + Y \]
\[ XY + M \rightarrow X + Y + M \]

**Bond rearrangement**

\[ X^+ + YZ \rightarrow XY^+ + Z \]
\[ X^+ + YZ \rightarrow X + YZ^+ \]
\[ X + YZ \rightarrow X + YZ \]

Interstellar and circumstellar conditions: chemical kinetics dominate

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021
Formation and destruction of molecules

Gas-phase chemistry

We know ion-molecule chemistry is important in disks because we see cations: \( \text{CH}^+, \text{HCO}^+, \text{N}_2\text{H}^+, \text{DCO}^+, \text{N}_2\text{D}^+, \text{YZ}^+ \)

Interstellar and circumstellar conditions: chemical kinetics dominate

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021
Formation and destruction of molecules

Grain-surface processes

Freezeout

Desorption

Dust grains act as a third body for association reactions

Formation and destruction of molecules

Dust grains act as a third body for association reactions

Grain-surface processes

Freezeout

Desorption

We know freezeout and desorption are important in disks because we see midplane depletion of e.g., CO, and gas-phase molecules present where they would otherwise be ice.

Dust grains act as a third body for association reactions

Formation and destruction of molecules

Grain-surface processes

Freezeout

Desorption

Hopping

Tunneling

Eley-Rideal

Langmuir-Hinshelwood

Dust grains act as a third body for association reactions

Formation and destruction of molecules

Grain-surface processes

- Gas-phase bombardment
- Sputtering
- H₂ formation
- Non-thermal desorption
- UV photons
- X-rays
- Cosmic rays
- Simple ices: H₂O:NH₃:N₂:CH₄:CO:CO₂:CH₃OH
- Energy → Heat
- Complex molecules

Formation and destruction of molecules

Burke, D. & Brown, W. 2010, PCCP, 12, 5947
We know grain-surface chemistry is important in disks because we see gas-phase molecules which are formed partly or solely on grain surfaces, e.g., CH$_3$CN and CH$_3$OH.
Grain-surface chemistry increases complexity

Grain-surface chemistry increases complexity

Calculating the chemistry

Molecular abundances are a function of disk conditions and time

\[ n_X = F \left[ T_{\text{gas}}, T_{\text{dust}}, n_{\text{gas}}, F_{\text{UV}}(\lambda), F_{\text{XR}}(E_{\text{XR}}), \zeta_{\text{CR}}, \sigma_{\text{dust}} \right] \]

\[ \frac{dn_X}{dt} = F_X - D_X \]

\[ \frac{dn_X}{ds} = F_X - D_X \]

\[ s = (r, z) \quad \text{or} \quad (\rho, \phi, z) \]

Chemistry in disks is not in equilibrium: steady state is possible
A “simple” chemical network: H$_2$

Dense gas:
Av $\gg$ 1 mag

\[ H_2 + \text{CR/XR} \rightarrow H_2^+ + e^- \]

Irradiated gas:
Av $< 1$ mag

\[ H_2 + \gamma_{\text{UV}} \rightarrow H + H \]

\[ H + H \rightarrow H_2 \]

A “simple” chemical network: $\text{H}_2$

**Dense gas:** 
$A_v \gg 1 \text{ mag}$

$\text{H}_2 + \text{CR/XR} \rightarrow \text{H}_2^+ + e^-$

**Irradiated gas:** 
$A_v < 1 \text{ mag}$

$\text{H}_2 + \gamma_{\text{UV}} \rightarrow \text{H} + \text{H}$

$\text{H}_2$ forms almost exclusively on dust grains

---

H⁺/H/H₂ in protoplanetary disks

H$^+$/H/H$_2$ in protoplanetary disks

X-rays also influence the H$^+$/H/H$_2$ transition regions

Increasing X-ray luminosity

Increase in H$^+$

Increase in H$_2$

A more complicated network: CO

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021
C\textsuperscript{+}/C/CO in protoplanetary disks

C\(^+\)/C/CO in protoplanetary disks

C\(^+\)/C/CO in protoplanetary disks

Similar stratification is seen in numerous physico-chemical models

ProDiMo

DaLI

An even more complicated network: H$_2$O

Grain-surface chemistry

Ion-molecule chemistry

“Hot” neutral-neutral chemistry

"Hot" neutral-neutral formed water

"Cold" ion-molecule/photo-desorbed water

Thermal desorption

Networks can quickly become complicated!

Creating synthetic observations

Absorption spectra at mid-IR

Hot dust

JWST

Creating synthetic observations

Radiative transfer codes (dust continuum and lines) are used along with molecular data to create synthetic spectra.

Absorption spectra at mid-IR

Hot dust

JWST

Creating synthetic observations

Emission spectra at (sub)mm

First detection of methanol (CH$_3$OH) in the disk around TW Hya

General outline of a physico-chemical model

- Laboratory data
- Quantum chemical calculations
- Astrophysical observations
- Physical assumptions
- Physical model
- Chemical model

Computing the chemistry

- Chemical abundances
- Molecular line radiative transfer
- Continuum radiative transfer

Compare and contrast

Simulated observations
General outline of a physico-chemical model

- Laboratory data
- Quantum chemical calculations
- Chemical model
- Physical model
- Astrophysical observations
- Physical assumptions

Computing the chemistry

- Chemical abundances
- Molecular line radiative transfer
- Continuum radiative transfer

Compare and contrast

Simulated observations
$T_{\text{gas}}$ and $T_{\text{dust}}$ decouple in disk atmosphere

At low densities and high ultraviolet fluxes, gas-grain collisions are inefficient and gas cools radiatively (which is slow)

Gas temperature calculation needs to be coupled with small chemical network to compute self-consistently the abundances of the main coolants: $[\text{Cl}]$, $[\text{OI}]$, CO, H$_2$O

Coupled physico-chemical models

**DALI**

Bruderer et al. (2012); Bruderer (2013)

**INPUTS**
- Density structure
- Stellar spectrum

**OUTPUTS**
- Spectra
- Image cubes

1. Continuum RT
2. Chemical network
3. Thermal balance
4. Excitation
5. Ray tracing

$T_{\text{dust}} < J_{\text{continuum}}$  
Atomic/molecular level population

Chemical networks for astrochemistry

Talk to an astrochemist!

Gas-phase chemistry
http://www.udfa.net/
http://kida.obs.u-bordeaux1.fr/
http://kinetics.nist.gov/kinetics/index.jsp

Photoionisation/photodissociation
http://home.strw.leidenuniv.nl/~ewine/photo/
http://phidrates.space.swri.edu/

Freezeout/desorption
Grain-surface chemistry
http://kida.obs.u-bordeaux1.fr/
http://faculty.virginia.edu/ericherb/research.html

Molecular data

Talk to an astrochemist!

LAMDA: Leiden Atomic and Molecular Database
http://home.strw.leidenuniv.nl/~moldata/

Cologne Database for Molecular Spectroscopy
http://www.astro.uni-koeln.de/cdms/

HITRAN/HITEMP
http://hitran.org/

JPL Molecular Spectroscopy
http://spec.jpl.nasa.gov/

ExoMol
http://www.exomol.com/
Radiative transfer codes

Talk to an astrochemist!

RADMC2D/3D
dust and lines
http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/

TORUS
dust and lines
https://www.astro.ex.ac.uk/people/th2/torus_html/homepage.html

RATRAN
lines
https://personal.sron.nl/~vdtak/ratran/frames.html

HYPERION
dust
http://www.hyperion-rt.org/

LIME
dust and lines
http://www.nbi.dk/~brinch/lime.php
Radiative transfer codes

Talk to an astrochemist!

RADMC2D/3D
http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/
dust and lines

RATRAN
lines
https://personal.sron.nl/~vdtak/ratran/frames.html

TORUS
dust and lines

HJPDOC
Dust optical constants
http://www.mpiia.de/HJPDOC/

HYPERION
dust
http://www.hyperion-rt.org/

LIME
dust and lines
http://www.nbi.dk/~brinch/lime.php
Future outlook

- Coupling dust evolution models with thermo-chemical and complex chemistry models: dust models are inherently 1D
- Correct treatment of viscous effects on disk structure and chemistry
- Large-scale mixing: connection with the solar system
- Breaking axisymmetry: creation of vortices, dust traps, and corresponding chemical effects
- Using molecular lines to distinguish between different models to explain dust morphology as observed with ALMA
- Chemistry in evolving disks: fingerprints of early conditions