Physical and Chemical evolution in protoplanetary disks

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Introduction: Protoplanetary disks (PPDs) around T-Tauri stars are thought to represent the formative stage of our own solar system. Understanding how these objects evolve chemically is necessary to understand the structure and development of our own solar system. Critical to this is proper consideration of the effect of dust grains. An understanding of their role in PPDs requires accurate modelling using the best available experimental and theoretical data, and observations directed and interpreted using such models.

This project aims to take an existing chemical model of the interstellar clouds and enhance it to more accurately model the chemistry of protoplanetary disks, with particular attention to the gas-grain interaction and deuterium fractionation. This will require the provision of accurate solid-phase laboratory data, particularly binding energies and reaction kinetics in ices, most of which will come from experiments currently being carried out by members of the LASSIE ITN.

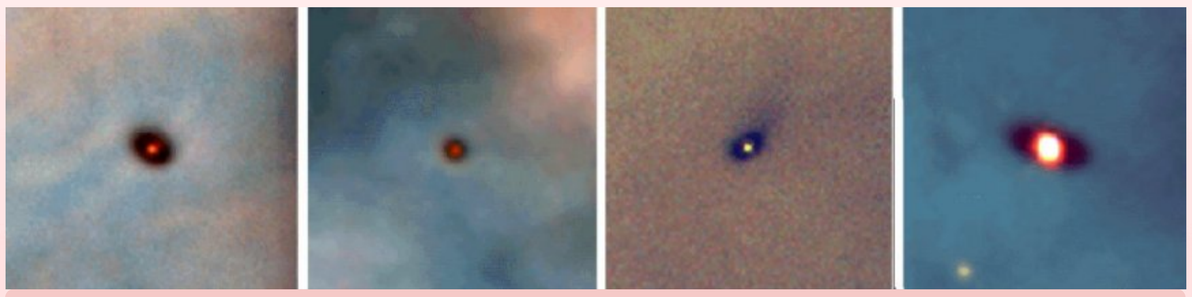

Figure 1: PPDs in the Orion nebula, imaged with the WFPC2 on the HST.

Role within the LASSIE ITN: This work is intended to:

- Refine the model currently in use with some of the changes outlined below.
- Use the laboratory data produced by experimental and theoretical members of the ITN to more accurately model protoplanetary disks, especially to quantitatively describe the role of dust grains in these objects. The new laboratory data and results of simulations will be used to improve:
  - Reaction networks – refining the lists of included reactions
  - Reaction data – better reaction rate coefficients and better data on temperature ranges over which they apply

The results of this improved model will be used to predict observational results and to use such results to constrain the effect of grain chemistry on PPDs.

Gas phase chemistry: Gas phase 2-body reactions* are typically modelled using the modified Arrhenius equation, which gives the reaction rate as a function of temperature. This is the preferred form for large reaction networks because they can be readily made into a network of coupled ordinary differential equations.

*At normal densities and temperatures in the ISM, 3 body collisions are sufficiently rare that we may neglect them.

Photochemistry and cosmic ray events: A PPD is subject to cosmic rays, the interstellar radiation field and irradiation by the central star. Each of these cause ionisation and dissociation. This may be modelled simply by specifying a flux, or by simulating the spectrum of the radiation field and treating each energy band differently. The intensity of the radiation must decrease with depth and radius, and self shielding which protects CO and H_2 from dissociation below the disk surface must be included.

Grains: Dust grains absorb and re-emit radiation, and gas phase molecules freeze onto them, altering the composition of the gas phase. Reactions which cannot occur in the gas phase can take place on the grain surface or in ice mantles. If these grains are later heated, these products are released and can be observable in the gas phase. If we wish to include the effects of grains, we must allow species to freeze onto the grain surfaces and to thermally desorb. We must also allow for desorption by non-thermal means such as cosmic rays and X-ray and UV photons.

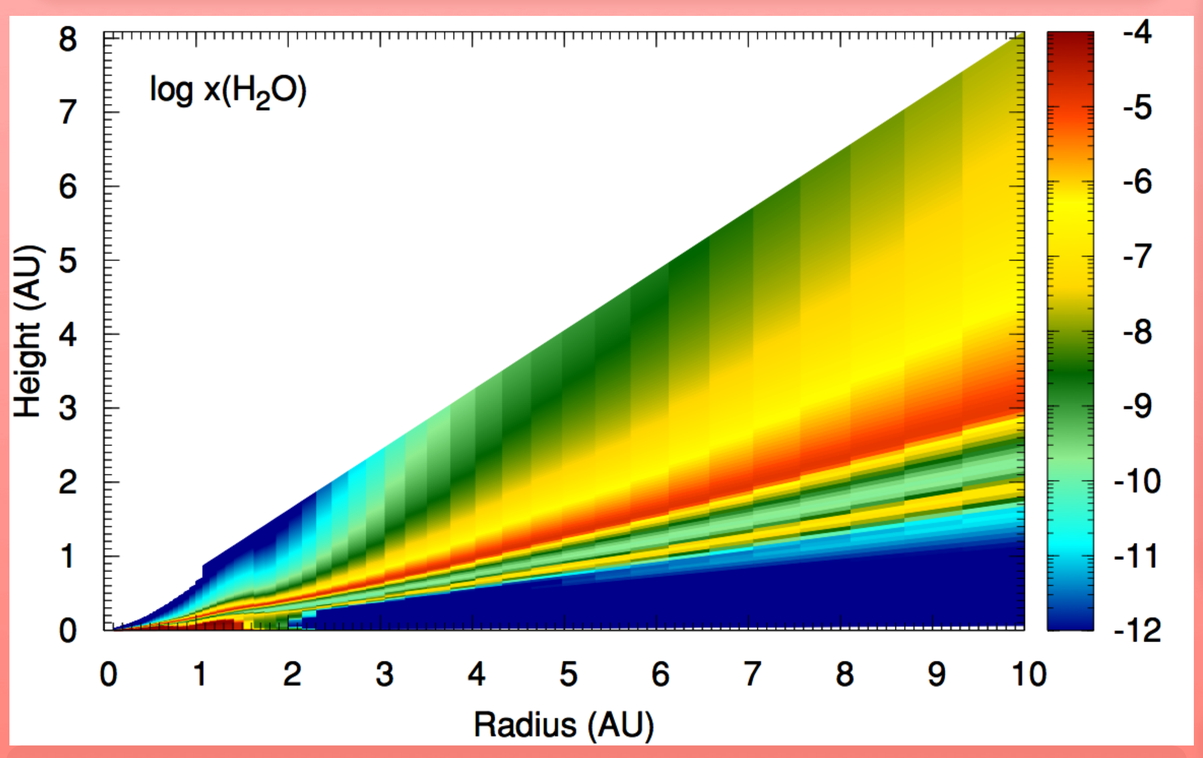

Figure 2: Gas phase abundance of H_2O in a PPD. Note the loss of water in the midplane due to freezing onto the grain surfaces. From [5]

Grain surface chemistry: Thermal diffusion over the grain surface is the key mechanism for surface species to meet and react.
For low mass particles quantum tunneling between sites enhances the reaction rates. Traditional approaches to surface kinetics can lead to unphysically high reaction rates due to the low number of reactants on a grain surface; clearly we cannot have a reaction between two grain surface species when one is not present on the grain. Per [2], we take the minimum timescale over which reactions take place to be either the accretion or evaporation timescale.
This may be refined further per [3] by allowing competition between processes.

Deuterium chemistry: Deuterium chemistry is essentially the only chemistry which proceeds in the gas-phase in cold, dense regions. In such conditions deuterium fractionation of some species can exceed the cosmic [D]/[H] ratio by several orders of magnitude.

Since deuterium bearing molecules are one of the only probes we have of the cold, dense midplane of PPDs – where planets and comets form – we have been incorporating its chemistry into our PPD model. We can compare model results of molecular [D]/[H] ratios with observations of comets to probe conditions in the early solar system.

Lacking experimental data on deuterium chemistry reaction rates, we may assume that these species as their hydrogen bearing analogues do.
This requires refinement; we must exclude reactions which are unphysical, and branching ratios must be calculated and applied to the reaction rates.
We must also take account of the modified masses of the deuterium bearing species for rates of desorption, diffusion and tunnelling.

Deuterium fractionation: There are approximately 30 basic reactions in which deuterium and hydrogen behave very differently, usually due to an energy barrier in one direction of a reversible reaction[4]. For example:
$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$
Has no activation energy in the forward direction, but a 180 Kelvin barrier to the back-reaction. Such reactions lead to certain species having [D]/[H] ratios greatly in excess of the cosmic ratio (10^{-5}:1) at low temperatures.

Spin isomers: Molecular hydrogen has two spin isomers, o-H_2 and p-H_2. Having different rotational energy levels means they will, in some cases, react differently. In particular, deuterium fractionation reactions have significantly different barriers and hence rate coefficients for the two spin isomers.

Modelling: Once the reaction set is assembled and the reaction rate coefficients are known, we have a set of first order ODEs. Providing initial values for chemical abundances (e.g. cosmic abundances) and integrating gives us the abundance of every species in the network as a function of time.

The model described so far is homogeneous. For a heterogeneous cloud we must model multiple points at the desired resolution. For a PPD, we can model a plane normal to the disk, intersecting the centre. Rotational symmetry allows us to use this for the whole PPD. The need to model thousands of sample points requires that the model be relatively efficient.

Networks of ODEs are computationally expensive to solve, limiting how much detail a model may have and still run in an acceptable time. Improved ODE solvers should reduce computing time to compensate for larger networks.

The model currently in use is derived from the model described in [5]. This model has also been adapted to simulate a range of objects, including disks around Herbig Ae stars

References:

[1]*Models of gas-grain chemistry in dense interstellar clouds with complex organic molecules*. Hasegawa, Herbst & Leung, ApJ, 1992
[2]*A proposed modification of the rate equations for reactions on grain surfaces.* Caselli, Hasegawa & Herbst, ApJ, 1998
[3]*A new modified-rate approach for gas-grain chemical simulations.* Garrod, A&A, 2008
[4]*Modelling of deuterium chemistry and its application to molecular clouds*, Roberts, A&A, 2000
[5]*Chemical processes in protoplanetary disks.* Walsh et al., ApJ, 2010

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