## The Gaseous Disks of Young Stellar Objects

A. E. Glassgold

Astronomy Department, University of California, Berkeley, CA 94720

aglassgold@astron.berkeley.edu

# ABSTRACT

Disks represent a crucial stage in the formation of stars and planets. They are novel astrophysical systems with attributes intermediate between the interstellar medium and stars. Their physical properties are inhomogeneous and are affected by hard stellar radiation and by dynamical evolution. Observing disk structure is difficult because of the small sizes, ranging from as little as 0.05 AU at the inner edge to 100-1000 AU at large radial distances. Nonetheless, substantial progress has been made by observing the radiation emitted by the dust from near infrared to mm wavelengths, i.e., the spectral energy distribution of an unresolved disk. Many fewer results are available for the gas, which is the main mass component of disks over much of their lifetime. The inner disk gas of young stellar objects (henceforth YSOs) have been studied using the near infrared rovibrational transitions of CO and a few other molecules, while the outer regions have been explored with the mm and sub-mm lines of CO and other species. Further progress can be expected in understanding the physical properties of disks from observations with sub-mm arrays like SMA, CARMA and ALMA, with mid infrared measurements using *Spitzer*, and near infrared spectroscopy with large ground-based telescopes. Intense efforts are also being made to model the observations using complex thermal-chemical models. After a brief review of the existing observations and modeling results, some of the weaknesses of the models will be discussed, including the absence of good laboratory and theoretical calculations for essential microscopic processes.

## 1. Introduction

Understanding how stars form is a natural development of several decades of study of molecular clouds, the birthplace of stars. A crucial stage in the process is the accretion phase, which involves several steps: the collapse of the nascent *molecular cloud core* (typical size about 0.1 pc), the formation of the *accretion disk* (extending in some cases from 0.05 AU to

1000 AU), and the development of *accretion flows* from the disk to the star and accompanied by outflows or winds from the inner regions of the disk. Starting from core collapse, the buildup of a low-mass star takes only a few million years, and the major accretion phase much less. Accretion is difficult to study because of the intrinsically inhomogeneous and dynamical nature of the dusty gas involved in the process. The observations require a multiwavelength approach that runs the gamut from X-ray to mm wavelength bands. The biggest observational obstacle to progress is the very small size of star-forming regions. Resolving a region of the size of our own planetary system (35 AU) at the distance of the nearby starforming cluster in Taurus (140 pc) requires a resolution of 0.25". Although such observations are possible in some of the relevant wavelength bands, imaging the most dynamic parts of the accretion process requires improvements in angular resolution of 1-2 orders of magnitude.

Theoretical modeling of accretion disks around low-mass stars in the process of formation presents its own challenges. Many of the simplifications used in interstellar cloud chemistry do not apply. For example, a common procedure in interstellar chemistry is to calculate the temporal evolution of hundreds of species at constant density under the assumption of complete photon shielding. This makes no sense for disks around YSOs because it is the irradiated surface regions that are usually observed. Not only is the assumption of complete shielding invalid for these regions, but account has to be taken of both the stellar and the interstellar radiation fields, each with its own spectral distribution. Even for an axisymmetric disk, the physical properties vary in both the radial and the vertical direction, so the assumption of a uniform medium is also invalid. In the rest of this report, After a brief review of the observations, I will try to give the flavor of the current state of theoretical modeling of the disks around low-mass YSOs, emphasizing some of the barriers to future progress, especially those involving the incompleteness of the underlying microscopic data.

#### 2. Observations of Disks

Most information about YSO disks comes from the spectral energy distribution (SED) which is dominated by emission from dust. SEDs are usually obtained by spatially-unresolved low-spectral resolution observations across the spectrum from near-infrared through mm wavelengths (made with several telescopes). A particularly interesting example (Lahuis et al. 2006) shown in Figure 1 includes *Spitzer* mid-infrared spectra as well as data from five other systems, 2MASS, VLT, ISO, SCUBA and IRAM. This is a rare case of a disk seen nearly edge on, so the silicate feature near  $10\mu$ m and various molecular features, both solid and gas phase, are seen in absorption.

Molecules are more often observed in emission from the optically thin surface regions of YSO disks, as reviewed at Protostars and Planets V (PPV, Najita, Carr, Glassgold & Valenti 2006; Dullemond et al. 2006). The main tool has been the ro-vibrational transitions of the abundant and robust CO molecule, although OH and  $H_2O$  have also been detected in



Fig. 1.— Composite SED of the edge-on disk around IRS 46 (Lahuis et al. 2006) from 1.25  $\mu$ m to 1,3 mm including the full *Spitzer* spectrum from 10-37  $\mu$ m (dark line). The light line is a theoretical model; the insert shows gas and solid molecular features.

the NIR. The absorption lines ascribed to  $C_2H_2$ , HCN, and  $CO_2$  in Figure 1 represent the first detection of polyatomic species in these disks, and much attention can be expected to be given to such species in the near future.

The most important result of the NIR observations of both the fundamental and overtone bands of CO (4.6  $\mu$ m and 2.3  $\mu$ m, respectively) is that the emission lines arise from warm gas (1000-1500 K) down to considerable depth ( $10^{21} - 10^{22}$  cm<sup>-2</sup>) in the inner disk (0.05 - 2.0 AU). Although well known for more massive YSOs (e.g., Najita et al. 1996 and references therein), Najita et al. (1993) have confirmed that they are a ubiquitous presence in the low-mass YSOs known as T-Tauri stars. The presence of the warm gas is confirmed by the detection of UV fluorescence from Ly- $\alpha$  pumped H<sub>2</sub> (e.g., Herczeg et al. 2002), also seen in many sources (reviewed by Najita et al. 2006 at PPV). The observation of the H<sub>2</sub> fluorescence provides a direct demonstration of the existence of vibrationally excited H<sub>2</sub> because the threshold for the excitation of the Lyman and Werner band electronic transitions from the ground state occurs at a shorter wavelength than Ly $\alpha$ .

The gas in disks can also be probed by mm and sub-mm transitions of CO, as has been demonstrated persuasively by observations with the IRAM Plateau de Bure interferometer and more recently at the SMA (reviewed at PPV by Guilloteau, Dutrey & Ho 2006). The difficulty here is that the available spatial resolution had been limited to about 1", but significant progress will be possible with the new generation interferometric arrays, such as SMA and CARMA, and eventually ALMA.

## 3. Thermal-Chemical Modeling

The goals and methodology of theoretical modeling of YSO disks are basically the same as for any astrophysical system: The abundance of the diagnostic species and the excitation of the upper level of a relevant spectral line need to be calculated. But this requires a knowledge of the physical properties, i.e., the density, temperature, and ionization fraction. For disks the physical properties themselves depend on the abundances, i.e., on the chemistry. Thus one needs to calculate the temperature and the abundances simultaneously in a selfconsistent manner. This kind of calculation is particularly challenging for disks because they are basically inhomogeneous with the physical properties varying over very wide ranges. An additional complication is that radiation fields of quite different character are involved, e.g., far ultraviolet (FUV) just below the H Lyman limit and X-rays with photon energies well above the ionization potential of H. For studying the inner disk, e.g., within 10 AU, the main source of the radiation is the young star itself, or from it's close environment such as the magnetosphere.

It is ironic that the X-ray properties of YSOs are better known than the FUV. The former has been studied with a series of X-ray observatories, such as ROSAT, Chandra and XMM-NEWTON, that are sensitive to the main band of YSO emission from 0.1 to 10 keV. On the other hand, HST cuts off at just before the crucial FUV band from 91 to 110 nm. Utilizing FUSE has helped, although there are problems (e.g., Bergin et al. 2003). Figure 2 shows an example of the X-ray spectrum of a YSO in the Orion Nebula Cluster observed with the *Chandra* COUP project (Getman et al. 2005). It shows how measured YSO spectra (highlighted by the solid line) are typically fit by two thermal components (lighter lines) with temperatures of order 1 keV and 3 keV. The hard component is responsible for the wide-ranging effects of X-rays incident on disks, e.g., the absorption length of a 3-keV X-ray photon is  $\sim 10^{23} \,\mathrm{cm}^{-2}$ . By way of contrast, a 100 nm FUV photon is absorbed over a column that is 200 times smaller. A significant fraction of the total luminosity of a low-mass YSO is emitted in X-rays, i.e.,  $L_X/L_{bol} \sim 10^{-4} - 10^{-3}$ . Thus for the nearby T-Tauri star TW Hya, only 56 pc distant,  $L_{\rm X} \sim 10^{30} \, {\rm erg \ s^{-1}}$ . The luminosity in FUV band from 91 to 110 nm is about the same (Bergin et al. 2003), but it is of course absorbed over a much smaller column. Another aspect of the UV emission of YSOs is the presence of a strong Ly $\alpha$  line, discussed above in the context of its role in exciting  $H_2$  flourescence; it's flux is typically 10% of the FUV flux from 91 to 110 nm. In principle, both X-ray and FUV radiation should be included in thermal-chemical modeling of YSO disks, but many of the papers in the literature tend to emphasize just one or the other.

Figure 3 shows vertical temperature profiles obtained by Glassgold, Najita, and Igea (2004; henceforth GNI04) with a thermal-chemical model based on the dust model of D'Alessio et al. (1999) for a generic T-Tauri star. The accretion rate is  $10^{-8} M_{\odot}$  and the radial distance is 1 AU. The gas temperature is plotted against perpendicular column density measured from the top of the atmosphere. The dashed line at the bottom shows the dust temperature rising above its midplane value due to the increase in illumination with height of small dust grains



Fig. 2.— X-ray energy spectrum of COUP source # 567 from Fig. 6b of Getman *et al.* (2005). The spectrum is fit (heavy solid line) by a conventional two-temperature model with  $kT_1 = 0.8 \text{ keV}$  and  $kT_2 = 3.1 \text{ keV}$  (lighter lines). The residuals present evidence of Ne-Fe anomalies often seen in strong flares. The sub-keV emission is absorbed out by intervening material with a column density,  $N_{\rm H} = 2 \times 10^{21} \text{ cm}^{-2}$ .

by the stellar radiation field. The dust undergoes a modest temperature inversion, going from about 140 K at midplane to 450 K at the top of the disk. Above a vertical column density  $\sim 10^{22} \text{cm}^{-2}$ , the gas temperature begins to depart from that of the dust and, due to strong surface heating, eventually manifests a very large temperature inversion high up in the atmosphere.

The figure contains several curves because GNI04 considered the possibility that the surface layers of protoplanetary disks are heated by the dissipation of mechanical energy as well as by stellar photons. This might arise through the interaction of a wind with the upper layers of the disk or through the effects of viscous dissipation associated with outward angular momentum transport. Since the theoretical understanding of these processes is incomplete, GNI04 adopted a phenomenological approach. The currently most widely accepted mechanism for viscous accretion is the magneto-rotational instability (Balbus and Hawley 1991; Stone et al. 2000), which leads to the local heating formula,

$$\Gamma_{\rm acc} = \frac{9}{4} \alpha_h \rho c^2 \Omega, \tag{1}$$

where  $\rho$  is the mass density, c is the isothermal sound speed,  $\Omega$  is the angular rotation speed, and  $\alpha_h$  is a phenomenological parameter that depends on how the turbulence dissipates. For example, one can argue, on the basis of simulations by Miller and Stone (2000), that midplane turbulence generates waves which, on reaching the diffuse surface regions, produce shocks and heating. Wind-disk heating can be represented by a similar expression on the basis of dimensional arguments. Equation 1 is essentially an adaptation of the expression



Fig. 3.— Temperature profiles from GNI04 for the surface of the protoplanetary disk atmosphere discussed in §3.1 of the text. The radial distance is 1 AU, and the mass-loss rate is  $10^{-8}M_{\odot}\text{yr}^{-1}$ . The dashed line is the dust temperature of D'Alessio *et al.* (1999). The solid curves are gas temperature profiles labeled by the coefficient  $\alpha$  in Eq. 1. The choice  $\alpha = 0.01$  closely follows the limiting case of pure X-ray heating. The abscissa is vertical column density in cm<sup>-2</sup>, and the ordinate is temperature in degrees K.

for the volumetric heating in an  $\alpha$ -disk model, where  $\alpha$  in general can depend on position. GNI04 used the notation  $\alpha_h$  to distinguish its role for heating the disk atmosphere with the phenomenological formula in Equation 1 (unfortunately, the subscript has been dropped from the figure).

The top layers of the atmosphere are fully exposed to X-rays, and the temperature there at 1 AU is ~5000 K. Further down, there is a warm transition region (500–2000 K), composed mainly of atomic hydrogen but with carbon fully associated into CO. The complete conversion from atomic H to H<sub>2</sub> is reached at a column density of  $6 \times 10^{21} \text{ cm}^{-2}$ , with more complex molecules such as water predicted to form deeper in the disk. The location and thickness of the warm molecular region depends on the strength of the surface heating. Thus X-ray heating dominates the transition region for  $\alpha_h < 0.01$ , whereas mechanical heating dominates when  $\alpha_h > 0.1$ . This result, that the warm transition region is mainly atomic hydrogen but has carbon fully associated into molecules, has the important consequence that CO rotation-vibration transitions are easily excited because of the large collisional excitation cross sections for H + CO inelastic scattering (much larger than for molecular hydrogen).

Gas temperature inversions can also be produced by UV radiation operating on small dust grains and PAHs, as demonstrated by the thermal-chemical models of Jonkheid et al. (2004), Kamp and Dullemond (2004) and Nomura and Millar (2005). Jonkheid et al. use the D'Alessio et al. (1999) model and focus on the disk beyond 50 AU. At this radius, the

gas temperature can rise to 800 K or 200 K, depending on whether small grains are well mixed or settled. For a thin disk and a high stellar UV flux, Kamp and Dullemond obtain temperatures that asymptote to several 1000 K inside 50 AU. Of course these results are subject to assumptions made about the stellar UV, the abundance of PAHs, and the growth and settling of dust grains. Nomura and Millar (2005) made a detailed thermal model of a disk that includes the formation of H<sub>2</sub> on grains, destruction via FUV lines, and excitation by  $Ly\alpha$  photons. The gas at the surface is heated primarily by the photoelectric effect on dust grains and PAHs (with a dust model appropriate for interstellar clouds, i.e., one showing little grain growth). Both interstellar and stellar UV radiation are included, the latter based on observations of TW Hya. The gas temperature at the surface of their flaring disk model reaches 1500 K at 1 AU. Their model partially account for the H<sub>2</sub> fluorescence measurements of Herczeg et al. (2002), although the theoretical fluxes fall short by a factor of five or so. A possible defect in their model is that the calculated temperature of the disk surface may be too low, a problem that might be remedied by reducing the UV attenuation by dust and by including X-ray or other surface heating processes. Disk chemistry was reviewed extensively at Protostars and Planets V by Bergin et al. (2006), Dullemond et al. (2006) and Najita et al. (2006)

### 4. Challenges for Laboratory Astrophysics

The initial attempts to model gaseous disks have had some success in understanding the warm atmospheric gas inferred from observations of CO and H<sub>2</sub>. Many other modeling challenges and opportunities await future observations of these and more complex species. The discussion in the previous sections shows that theoretical modeling is complicated. It is also fraught with uncertainties and ambiguities characteristic of our limited understanding of YSO disks. Much of the uncertainty comes from the unknown (and time-dependent) gas distribution and from our poor understanding of how disks are heated. Rather than focusing here on these astrophysical issues, we highlight the gaps in the microphysical basis of thermal-chemical modeling. Although we mainly referred to our own calculations in §3 for purposes of illustration, there is almost universal agreement on the laboratory astrophysics needs of modelers of YSO disks.

### 4.1. Gas Phase Reactions

The occurence of a chemically active transition zone between hot and cold gas layers clearly indicates that, at least in the inner regions of disks, neutral radical reactions are essential for understanding disk chemistry. Modeling of disks involves temperatures that range below 500 K. Since most neutral reactions have activation energies, their rate coefficients are small in this temperature range, and they are difficult to measure, especially radicalradical reactions. A good example is the well-studied reaction,  $O + H_2 \rightarrow OH + H$ , important for the synthesis of CO and H<sub>2</sub>O. Most modelers agree on the rate coefficient above 500 K, but disagree at lower temperatures. The experiments in this temperature range are typically 30 years old. Two other consideration are relevant. First, the inverse reaction, OH + H $\rightarrow O + H_2$ , is also important, but its rate coefficient has not been measured and has to be calculated from detailed balance; again, there is considerable uncertainty in its value at low temperature. Second, the fine structure of the O atom becomes important in this temperature range. Sims et al. (2006) have taken up this challenge in a number of interesting cases. Similar considerations apply to S atom reactions, for which measurements are badly needed.

Another class of poorly known reactions affecting disk chemistry is low-energy  $(< 1 \, \text{eV})$ charge exchange. Mutiply-charged heavy ions are produced by hard ( $\gtrsim 1 \, \text{KeV}$ ) X-rays via the Auger effect. Disk gas is incompletely ionized, and the abundance of atomic hydrogen is large in the atmosphere exposed to X-rays. The higher ions rapidly charge transfer to H, but the rate coeffcients for low ions are poorly known at low temperatures. The case of S was discussed at the last workshop (Glassgold 2002). The ions  $S^{q+}$  with q = 3 - 6 are produced by keV stellar X-rays. The high-level calculation of Stancil et al. (2001) shows that  $S^{4+} + H \rightarrow S^{3+} + H^+$  is fast down to low temperatures, but the situation for  $S^{3+}$  and  $S^{2+}$ remains problematic. Early calcuations of  $S^{2+} + H \rightarrow S^+ + H^+$  (Butler & Dalgarno 1980, Christensen & Watson 1981) suggest that the rate coefficient is small at low temperatures. Calculations of  $S^{3+}$  charge exchange (Bacchus-Montabonel 1998; Labuda et al. 2004) are restricted to keV energies. The recent study of  $H^+ + S \rightarrow S^+ + H$  by Zhao et al. (2005) sheds new light on the temperature variation of this important reaction. Theoretical and experimental studies of  $S^{2+}$  and  $S^{3+}$  charge transfer with H at low energies are badly needed. These essentially unknown rates affect the abundance ratio SII/SI and thus the intensities of both optical/infrared forbidden and mid-infrared fine structure transitions from disks and jets. Similar gaps in low-energy charge exchange rate coefficients are common among the ions of other heavy elements.

Many if not most of the reactions needed by chemical modelers have not been studied experimentally or theoretically. This is a serious problem since literally thousands of reactions are potentially important. In the case of ion-molecule reactions, approximate rules hold in many cases, at least when the reactions are highly exothermic. But general rules are more difficult to obtain for neutral reactions, especially at very low tempertaures. A similar statement applies to charge transfer reactions below 1 eV, as just discussed. A useful response to this situation is to identify the handful of reactions that are truly critical in a particular problem and to then make the case for experimental measurement. Of course some modelers have always chosen to work with small selected sets of reactions. More recently, several groups have attempted to determine the crucial reactions for particular problems by objective criteria and to assess the effect of rate coefficent uncertainties on modeling results (e.g., Wiebe, Semenov, & Henning 2003; Semenov, Wiebe, & Henning 2004; Wakelam et al. 2005). The Munich group has focused on the implications for disk modeling (Semenov, Wiebe, & Henning 2004; Semenov, Henning, & Vasyunin 2006, private communication). They find that the largest effects of uncertainties in rate coefficients are radical-radical reactions near the midplane and radiative-association reactions above the midplane.

#### 4.2. Dust and PAHs

Grain surface chemistry almost certainly plays a critical role in disks because of the high density and the low temperatures near the midplane. Not too close to the star, the temperature are low enough to condense volatile species, even those with small dipole moments such as CO. Granted that freeze-out is likely to occur, we need to understand what kinds of reactions occur on grain surfaces and how the products are removed. It is generally assumed that a one result of grain surface chemistry is the hydrogenation of heavy atoms and radicals, leading for example to the production of ammonia and methane. More complex reactions occur that are crucial for understanding the chemical environment of disks in the region of planet formation. All of the disk modelers contacted for this review agree that laboratory experiments and theoretical simulations of adsorption and desorption processes (especially photodesorption) as well as surface reactivity are among the most important needs of disk chemistry. Further studies of molecular hydrogen formation on surfaces would also be of great interest, e.g., by going to higher temperatures and including deuterium reactions.

A similar consensus recommendation applies to PAHs, which have been observed in disks. If their abundance turns out to be similar to that found in the interstellar medium ( $\sim 10^{-7}$  relative to total hydrogen), then PAHs obviously have a role to play in the ionization and chemistry of YSO disks. The role of PAHs in the heating of disks is clearly demonstrated by the calculations of Nomura & Millar (2005), referred to in §3. Another aspect of PAHs in disks that merits laboratory study is the effect of X-rays on their chemical structure and abundance. Among the basic chemical processes of PAHs that need further investigation are electron attachment, photoionization and neutralization.

#### 5. Conclusion

We have tried to show that improving observational capabilities will soon begin to reveal the distribution of the gas in the disks of YSOs, and that this will contribute significantly to our understanding of how low-mass stars form. Detailed thermal-chemical modeling of the physical properties of the disks will be required to interpret the observations. But the astrophysics of the disks calls for complex models and, to obtain meaningful results, significant uncertainties in the underlying physical and chemical processes need to be reduced by theoretical and laboratory studies. Work is particularly needed on the following topics:

- 1. Dust surface chemistry
- 2. PAH structure, spectroscopy and chemical kinetics
- 3. Gas phase neutral radical reactions and radiative association
- 4. Ionic reactions of atoms and radicals, including charge exchange of 1st and 2nd ions
- 5. Photo processes, including photodissociation and especially photodesorption from grains
- 6. X-ray interactions with dust grains and PAHs
- 7. Collisional excitation rates
- 8. Critical evaluation and maintenance of reaction rate data bases

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