X-RAY—IRRADIATED PROTOPLANETARY DISK ATMOSPHERES. I. PREDICTED EMISSION-LINE SPECTRUM AND PHOTOEVAPORATION

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ABSTRACT

We present mocassin two-dimensional photoionization and dust radiative transfer models of a prototypical T Tauri disk irradiated by X-rays from the young pre-main-sequence star. The calculations demonstrate a layer of hot gas reaching temperatures of ~10⁴ K at small radii and ~10⁵ K at a distance of 1 AU. The gas temperatures decrease sharply with depth, but appear to be completely decoupled from dust temperatures down to a column depth of ~5 × 10²¹ cm⁻². We predict that several fine-structure and forbidden lines of heavy elements, as well as recombination lines of hydrogen and helium, should be observable with current and future instrumentation, although optical lines may be smothered by the stellar spectrum. Predicted line luminosities are given for the brightest collisionally excited lines (down to ~10⁻⁸ L☉) and for recombination transitions from several levels of H i and He i. The mass-loss rate due to X-ray photoevaporation estimated from our models is of the order of 10⁻³ M☉ yr⁻¹, implying a dispersal timescale of a few Myr for a disk of mass 0.027 M☉, which is the mass of the disk structure model we employed. We discuss the limitations of our model and highlight the need for further calculations that should include the simultaneous solution of the two-dimensional radiative transfer problem and the one-dimensional hydrostatic equilibrium problem in the polar direction.

Subject headings: accretion, accretion disks — infrared: stars — planetary systems: protoplanetary disks — stars: formation — stars: pre–main-sequence — X-rays: stars

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1. INTRODUCTION

Protoplanetary disks are a product of the formation of protostars from the collapse of molecular cloud cores. These disks remain a source of ongoing accretion for the central stellar object for a period of up to ~10 Myr (Manning & Sargent 1997; Wyatt et al. 2003) and are the birthplaces of planetary systems. The evolution of the disk and of its planetary progeny is controlled by heating and irradiation from the central star, from IR to X-rays, but in the vicinity of OB stars it can also be significantly affected by the external radiation environment (e.g., Johnstone et al. 1998; Adams et al. 2004; Fatuzzo & Adams 2008).

The discovery of the proplyd phenomenon and subsequent observations of protoplanetary disks represent an important and growing part of the legacies of the observations of protoplanetary disks. Pioneering work from the Hubble Space Telescope and the Spitzer Space Telescope (e.g., O’dell 1993; Bally et al. 1998; Evans et al. 2003; Meyer et al. 2004). New instruments such as the Mid-Infrared Instrument on board the James Webb Space Telescope, which will provide both imaging and spectroscopy, hold the promise for higher spatial resolution. On the ground, millimeter and submillimeter studies have evolved from examining disk size and orientation (e.g., Keene & Masson 1990; Lay et al. 1994) to detailed studies of structure, chemistry, and thermal properties (e.g., Wilner et al. 2003; Qi et al. 2006), while future high spatial resolution submillimeter observations with the Atacama Large Multimeter Array (ALMA) promise further major advances (e.g., van Dishoeck & Jørgensen 2008).

These and other observations should provide insights into issues central to understanding disks and the likelihood of forming planetary systems like our own, such as angular momentum transport, and the timescales for grain growth and gas dissipation. Of particular interest for interaction of the disk with its parent star and for the study of planetary origins are the inner regions of disks (≤10 AU), where both terrestrial and giant planets are believed to form.

While the observational database continues to grow, all attempts at theoretically modeling the emission expected from such environments have lacked several of the ingredients needed for a fully self-consistent approach. The multidimensional, far-ultraviolet (UV) to X-ray radiative transfer (RT) problem must be solved simultaneously with the disk hydrodynamical evolution, to which it is strongly coupled. Furthermore, disks comprise adjacent regions of ionized, photon-dominated, and molecular gas intermixed with a nonuniform dust component. No computer code currently available includes all the important physics and chemistry needed to properly interpret the observational diagnostics of these different regimes. Furthermore, full theoretical understanding of a number of important contributors to the energetics of the system, such as accretion and wind-disk interactions, is still lacking; these ingredients can currently be included only through approximate and phenomenological approaches (e.g., see discussion in GNB04).

Several studies have focused on the properties of the dust component of disk atmospheres (e.g., D’Alessio et al. 2001; Dulmond et al. 2002; Akeson et al. 2005). However, studies of the gaseous component of the inner disks have only recently been attempted, and only an exploratory picture of the thermochemical structure of this crucial component has emerged. Pioneering work from Igea & Glassgold (1999), GNB04, Glassgold et al. (2005), and Meijerink et al. (2008, hereafter MGN08) examined physical conditions and expected emission lines in the gaseous component of non-evolving T Tauri disks irradiated by X-rays. Nomura & Millar (2005) modeled molecular hydrogen emission from protoplanetary disks, taking into account UV radiation from a central star;
their models, while calculating the density and temperature structures self-consistently, did not account for X-radiation and employed an approximate treatment of the scattered light that often leads to an overestimation of the UV radiation field in the disk (Glassgold 2006). Semenov et al. (2004) employed perhaps the most complete chemical network to date to calculate the ionization fractions at the disk midplane. While X-ray ionization was included, radiative transfer through scattering and diffusion was not. Simple column density arguments were used instead to estimate the radiation field attenuation at discrete points in the disk where the chemical model was applied. Very recently, Gorti & Hollenbach presented one plus one-dimensional models of gas in optically thick disks, calculating thermal, density, and chemical structures, with special attention to the effects of FUV irradiation.

More detailed two- or three-dimensional calculations are now needed to provide a quantitative picture of these environments in relation to their effects on the disk spectral energy distribution (SED) and on other observables available now and in the near future (e.g., [O i], [Ne ii], CO, OH, and UV transitions of H$_2$; Najita et al. 2007).

In particular, observations of forbidden lines in T Tauri stars provide evidence for a tenuous, hot outer layer, or “corona” (Kwan & Tademaru 1988, 1995; Kwan 1997). The earlier work by GNI04, Glassgold et al. (2007), Semenov et al. (2004), and MGN08 emphasized the chemistry in the photodissociation region (PDR) and molecular zones, stopping short of this coronal layer. In addition, the recent work by Gorti & Hollenbach does not include the fully ionized layer discussed here.

In this paper, the first of a series aimed at building a more realistic and self-consistent model of irradiated gaseous T Tauri disks, we employ a fully three-dimensional photoionization and dust radiative transfer code, moca/bin (Ercolano et al. 2003, 2005, 2008), to calculate the detailed ionization and temperature structure of a typical T Tauri disk, with special emphasis on the photoionization-dominated outer layers and corona. We show that hot coronal temperatures are expected from X-ray irradiation from the central pre–main-sequence star. Our calculations aim to explain the thermochemical structure of the irradiated region and to identify emission lines that can be used as gas-phase diagnostics for current and future observations. Furthermore, the detailed two-dimensional temperature structure calculated by our models allows us to estimate the efficiency of X-radiation to drive a photoevaporative wind.

Our model is described in § 2. The ionization and temperature structures are presented and discussed in § 3, while the predicted emission-line spectra are shown in § 4. Section 5 contains a discussion of our results in the context of disk dispersal via X-ray photoevaporation. A brief summary is given in § 6.

2. THE TWO-DIMENSIONAL MONTE CARLO PHOTOIONIZATION AND DUST RADIATIVE TRANSFER MODEL

Photoionization and temperature structure calculations were performed with version 3.0.2.0 of the three-dimensional Monte Carlo photoionization and dust radiative transfer code, moca/bin (Ercolano et al. 2003, 2005, 2008). The code uses a stochastic approach to the transfer of radiation allowing for the self-consistent transfer of both the primary and secondary components of the radiation field. The code was modified to include viscous heating, approximated using the prescription for a thin disk by Pringle (1981), and gas cooling by collisions of grains with a mixture of atomic and molecular hydrogen (Hollenbach & McKee 1979); we discuss this further below. The code moca/bin was also adapted to run in two dimensions, using the gas and dust density distribution given by a two-dimensional protoplanetary disk calculation of D’Alessio et al. (1999).

The D’Alessio model used in our calculation was chosen to be the one that best fits the median SED of T Tauri stars in Taurus (D’Alessio 2003). We refer the reader to D’Alessio et al. (1999) for a detailed description of the model ingredients and calculation. In brief, the input parameters for this model include a central star of 0.7 $M_\odot$, 2.5 $R_\odot$, irradiating the disk with an effective temperature of 4000 K. Additional disk parameters consist of a mass accretion rate of $10^8 M_\odot$ yr$^{-1}$ and a viscosity parameter $\alpha = 0.01$. The total mass of the disk is 0.027 $M_\odot$.

The present study is particularly focused on determining the physical properties of the gas in the outer layers and hot-disk corona. Molecular species that are expected to form deeper in the disk are not included in our model; this poses a limitation on the accuracy of our gas temperature calculations in the inner layers. In particular, the calculations by GNI04 have shown that CO rovibrational lines may become important coolants, and, e.g., at a radial distance of 1 AU and column densities of $10^{21}$–$10^{22}$ cm$^{-2}$, CO was found to dominate the disk cooling. CO rotational lines are also expected to form at greater depths, although in these regions the thermal balance is dominated by dust-gas collisions (GNI04).

Dust-gas collisions can heat the gas/dust if the gas is cooler/warmer than the dust; photoelectric emission from dust grains heats the gas, and it provides a minor cooling channel for the dust. The code moca/bin is able to self-consistently calculate the dust and gas thermal balance, taking into account the main microphysical processes that couple the two phases. Here, however, we choose to keep the dust temperatures fixed to the values calculated by D’Alessio et al. (1999) and focus our discussion on the gas phase. In the current work, we do not treat the transfer of the stellar or interstellar far-UV field, and therefore the dust temperatures we would obtain from our models would be incorrect. The effects of gas-dust interactions on the temperature structure of the gas, however, are still taken into account in our gas thermal balance, as well as in the radiative transfer, where the competition between dust and gas for the absorption of X-ray radiation is properly treated.

We illuminate the disk using synthetic X-ray spectra representative of the high-energy emission from a typical T Tauri star. There are currently at least three different mechanisms by which T Tauri stars are thought to produce observable X-rays: magnetospheric accretion shocks, shocks resulting from polar jets, and magnetically confined hot corona analogous to those found on all late-type main-sequence stars, including the Sun (e.g., Kastner et al. 2002; G"udel et al. 2005; Walter & Kuhl 1981). The first two of these have been identified only in a small handful of stars, and since the latter appears to dominate the observed X-ray spectra of T Tauri stars, we currently ignore the effects of X-rays from jets and accretion.

Coronal X-ray emission arises from an optically thin plasma dominated by impact excitation and ionization by thermal electrons. The spectra from such a plasma comprises significant contributions from bound-bound, bound-free, and free-free radiation. We computed synthetic coronal spectra incorporating these processes for the energy range 13.6 eV–12.5 keV for all elements with atomic number $Z = 1$ to 30 using line and continuum emissivities from the CHIANTI compilation of atomic data (Landi & Phillips 2006, and references therein), together with ion populations from Mazzotta et al. (1998), as implemented in the PINToFALe IDL software suite (Kashyap & Drake 2000). We adopted the solar
The dust absorption and scattering coefficients are calculated for high energies using the dielectric constants for graphite and silicates of Laor & Draine (1993), which extend to the X-ray domain. We assume spherical grains and use standard Mie scattering series expansion for \( \chi < 1 \), where \( \chi \) is the complex refractive index and \( x = 2a/\lambda \) is the scattering parameter (see Laor & Draine 1993). For \( \chi > 1000 \) and \( \chi - 1 < 0.001 \), we use Rayleigh-Gans theory (Bohren & Huffman 1983), and for \( \chi > 1000 \) and \( \chi - 1 > 0.001 \), we use the treatment specified by Laor & Draine (1993), which is based on geometric optics.

Our dust model consists of a typical interstellar medium (ISM) mixture of graphite and silicates with a Mathis, Rumpl, and Nordsieck (MRN) size distribution (Mathis et al. 1977) described by \( a_{\text{min}} = 0.005 \mu m \) and \( a_{\text{max}} = 0.25 \mu m \). The chosen grain size distribution does not take into account grain growth and therefore overemphasizes the cooling of the gas by the dust in the disk interior. We also assume a dust-to-gas mass ratio of 0.01 throughout the disk. We note that the density distribution model of D’Alessio et al. (1998) uses different dust prescriptions at different heights, in order to account for the effects of grain settling and growth. For the sake of simplicity and because we assume the dust temperatures calculated by D’Alessio et al. (1998), we chose to use a more standard dust model throughout our disk. Since matching a particular SED is not one of our main objectives and we are mostly interested in the physical properties of the disk corona, the choice

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\text{Note.—The flux at a distance } D, \text{ assuming a face-on orientation of the disk, is obtained by dividing the line luminosities by } 4\pi D^2.
\]
of the size distribution and species is not crucial in our work, as it will have only a very small effect on the ionization and temperature structure of the coronal gas.

As noted earlier, in addition to all the standard heating and cooling channels included in mocassin, we also include viscous accretion heating calculated assuming the standard dissipation rate for a thin disk (Pringle 1981)

$$\Gamma_{\text{acc}} = \frac{9}{4} \alpha \rho c_s^2 \Omega,$$

where $\rho$ is the local mass density of the gas, $c_s$ is the isothermal sound speed, and $\Omega$ is the angular rotation speed. The parameter $\alpha = 0.01$ relates viscous heating to the gas pressure.

The formulation above is purely phenomenological and carries large uncertainties. In particular, the appropriate value of $\alpha$ is unclear when the formula is applied to the warm-disk atmosphere (GNI04), where it is unknown whether angular momentum transport, such as the magnetorotational instability (MRI; Balbus & Hawley 1991), even operates at all. GNI04 show the effect that varying the value of $\alpha$ has on the temperature structure of the gas, but finally adopt a model with $\alpha = 0.01$ for their line emission predictions (Glassgold et al. 2007; MGN08). A value of $\alpha = 0.01$ is also chosen by D’Alessio et al. (1998, 1999, 2001) for their disk structure calculations (which include the model used in this paper). This choice is based on the connection between $\alpha$ and the disk accretion rate, $\dot{M}_D \propto \alpha \Sigma_D$, where $\Sigma_D$ is the integrated surface density of the disk. With $\alpha = 0.01$, which is also the value implemented in our models, X-ray heating is dominant in the disk corona, while accretion heating dominates in the inner regions.

We finally note that the dependence of the heating rate on the square of the sound speed implies a linear dependence on the gas temperature, which poses potential problems for the hot-disk corona. In the regions where the gas is heated to high temperatures by X-ray irradiation, the functional form of accretion heating, as formulated above, fails completely, preventing an equilibrium temperature from being found. In fact, X-ray irradiation in the upper atmosphere of the inner regions of the disk heats the gas to temperatures above the local escape temperature of the gas (see § 5). The gas in these regions is to be considered unbound and part of a photoevaporative flow, hence not subject to the standard viscous accretion law. For unbound gas, we remove the accretion heating contribution altogether by setting the local $\alpha$-coefficient to zero in our models.

3. THE IONIZATION AND TEMPERATURE STRUCTURE

In this section, we present the temperature and ionization structure of the gas in the inner disk, focusing our attention on the disk corona. We limit our discussion to radial distances $R \lesssim 40$ AU, beyond which, in our model, sets a rough outer limit to the region where the effects of X-ray irradiation on the temperature and ionization structure are more evident. We note, however, that in our models, a low level of ionization is maintained out to a radius of $\sim 190$ AU.

Figure 1 shows the temperature structure (asterisks) in the vertical column calculated at $R = 0.07$ AU, together with the dust temperature profile calculated by D’Alessio et al. (1999). Also shown is the volumetric gas density (cm$^{-3}$) as a function of depth; the corresponding geometrical height above the midplane is shown in the top x-axis. The gaseous disk corona at these very small radii is fully ionized. Since all elements are stripped of their outer electrons, cooling by collisionally excited lines is inefficient. The balance between heating by photoionization and cooling by line emission and recombination processes corresponds to a gas equilibrium temperature of $\sim 10^6$ K.

At 0.07 AU, the jump in gas temperature occurs at a vertical column density of $\sim 5 \times 10^{14} \text{ cm}^{-2}$, where the gas density is $\sim 3 \times 10^4 \text{ cm}^{-3}$ and the ionization parameter, defined as $\xi = L/nR^2$, is log $\xi \sim 1.78$. This transition would look even sharper in a hydrostatically balanced model, since a rise in the temperature would induce a drop in density in order to maintain pressure equilibrium. In this case, any equilibria found in the $10^4$–$10^6$ K range may in fact be unstable (Hatchett et al. 1976). This has already been noted in accretion disk models around X-ray binaries (e.g., Raymond 1993). Alexander et al. (2004, hereafter ACP04) have also presented a model to illustrate the effects of X-ray heating on the structure of circumstellar disks.

In that work, the density profile was truncated at the point where the density fell to $10^5 \text{ cm}^{-3}$, which is below the fully ionized region shown in our Figure 1. This should be kept in mind when comparing our temperature structure to theirs (as shown in their Fig. 3), where the lack of the $\sim 10^6$ K temperature (fully ionized) region is not surprising and is not discrepant with our results.

The electron density distribution, shown in Figure 2, indicates that the high level of ionization at 0.07 AU is maintained for a column density of $10^{17} \text{ cm}^{-2}$, after which it decays to lower
X-ray heating dominates for a column depth of \(10^{18}\) cm\(^{-2}\). A study of the thermal balance at this radius indicates that in the disk, where it is balanced by dust-gas collisional cooling. In our calculations, the contribution from accretion heating is set to zero in regions where X-ray irradiation heats the gas to temperatures above the local escape temperature (see § 2). At \(R = 0.07\) AU, this occurs at a column depth of \(10^{14.5}\) cm\(^{-2}\), at the onset of the temperature discontinuity.

Figure 3 shows the temperature and volumetric density (cm\(^{-3}\)) structures in the vertical column calculated at \(R = 1\) AU, together with the D’Alessio et al. (1999) dust temperature profile. The coronal gas here appears to be only partially ionized, and the electron density, illustrated in Figure 4, reaches a level of just over 10% of the hydrogen density, but decreases very rapidly with column depth.

Our temperature structure at 1 AU is comparable to that found by GNI04, allowing for differences in the model input parameters and bearing in mind that their calculation started at a column depth of \(10^{18}\) cm\(^{-2}\). However, the cooling and heating contributions calculated by these models disagree somewhat and deserve further explanation. The various heating and cooling channels in our model at 1 AU are illustrated as a function of vertical column depth in Figure 5, which can be compared with an analogous illustration in Figure 3 of GNI04. One conspicuous difference between the two models is the accretion heating contribution, which is simply due to the different choice of \(\alpha\). Note that GNI04 also investigated models with lower values of \(\alpha\) (see their Fig. 2) and indeed used a model with \(\alpha = 0.01\) for their later work (Glassgold et al. 2007; MGN08), in which emission-line predictions are given. Unfortunately, a plot showing the heating/cooling contributions from their models is available only for the \(\alpha = 1\) case. Another important difference lies in the Ly\(\alpha\) cooling contribution, which is of only secondary importance in our models, but dominates the cooling down to a vertical column of \(10^{21}\) cm\(^{-2}\) in the GNI04 model. The dominant cooling mechanism in the upper disk atmosphere in our model is metal line emission. The Ly\(\alpha\) cooling in GNI04 was overestimated, because of an assumption of a thermal equilibrium population for the \(n = 2\) level. The Ly\(\alpha\) channel in the GNI04 model also includes cooling by the fine-structure lines of O \(\text{I}\), while other atomic coolants are ignored. In spite of the aforementioned differences, the total cooling calculated by GNI04 is very similar to that obtained in this work for the regions where the calculations overlap and when the same \(\alpha\)-parameter is employed (A. E. Glassgold 2008, private communication).

As we move to increasingly larger radii, up to approximately 25–30 AU, our model disk structure remains qualitatively similar to that at 1 AU: high gas temperatures are reached in the corona, followed by a steep temperature decrease, with the gas and dust becoming thermally coupled at a vertical column depth of \(\sim 5 \times 10^{21}\) cm\(^{-2}\). Beyond \(\sim 35–40\) AU, due to geometrical dilution of the central radiation field, the effects of X-ray irradiation become less evident; however, a low level of ionization is maintained out to a radius of \(\sim 190\) AU. For \(\tau\) Tauri stars born in clusters containing massive stars, such as the Orion Nebula cluster, the dominant irradiation mechanism at large disk radii is probably provided by the interstellar or intracluster FUV and X-ray fields, which are not included in our current models. This is not true for stars born in smaller clusters such as \(\rho\) Ophiuchi and Taurus-Auriga, where indeed large disks (\(\sim 500–1000\) AU) are found (Andrews & Williams 2007).
The maximum temperature reached by the disk corona at a given radial distance is an immediate consequence of the local ionization parameter. The fact that at 1 AU we do not see the \( \sim 10^5 \) K gas layer is simply due to the fact that the density distribution of D’Alessio et al. (1999) used in our models is truncated at a volumetric density of \( \sim 10^4 \). At 0.07 AU, the temperature jump to \( \sim 10^6 \) K occurs at log \( \xi \sim 1.78 \). The same value at 1 AU implies a density of \( \sim 150 \) cm\(^{-3} \), which is below the cutoff. The general results found in our models are similar to those found by Gorti & Hollenbach (2008), in particular that the gas and dust are thermally decoupled down to a column of \( \sim 10^{22} \) cm\(^{-2} \).

4. PREDICTED EMISSION-LINE SPECTRUM

As an aid to future observational campaigns, we have calculated the emission-line spectrum predicted by our model. Line luminosities are integrated out to a radius of 190 AU. In Tables 1 and 2 we list a subset of the strongest collisionally excited metal line and hydrogen recombination lines, respectively, down to a luminosity of \( \sim 10^{-8} \) \( L_\odot \), which corresponds to a flux of \( \sim 1.8 \times 10^{-17} \) ergs s\(^{-1} \) cm\(^{-2} \) at a distance of 140 pc. The flux at a distance \( D \), assuming a face-on orientation for the disk, is obtained by dividing the line luminosities by \( 4\pi D^2 \).

A number of potential atomic and ionized gas diagnostic lines should already be detectable with current instrumentation. The [Ne \( ii \)] 12.8 \( \mu m \) line, in particular, has already been detected in T Tauri disks with Spitzer by Pasucci et al. (2007), Lahuis et al. (2007), and Espaillat et al. (2007), and with MICHELLE on Gemini North by Herczeg et al. (2007). The detections to date range from a few \( 10^{-7} \) to \( 10^{-5} \) \( L_\odot \), in qualitative agreement with values predicted by our model. The [Ne \( iii \)] 15.5 \( \mu m \) line has so far been detected only in Sz 102 (Lahuis et al., 2007), implying a [Ne \( iii \)]/[Ne \( ii \)] of \( \sim 0.06 \) for this object, which is some 2.5 times larger than our model. As noted by Glassgold et al. (2007), the abundance of Ne\(^{3+} \) is lowered by charge exchange reactions with neutral H, implying low (\( \leq 0.1 \)) ratios of [Ne \( iii \)]/[Ne \( ii \)] in the X-ray-heated gas. Gorti & Hollenbach (2008) also discuss the effects of EUV irradiation that would enhance the predicted [Ne \( ii \)] and [Ne \( iii \)] line luminosities and affect their ratio. They predict that the [Ne \( iii \)]/[Ne \( ii \)] ratio also depends on the details of the EUV spectrum, with hard EUV spectra naturally producing the higher ratios.

Table 1 clearly shows that a number of optical lines have fluxes that are significantly larger than the [Ne \( ii \)] 12.8 \( \mu m \) fluxes. Unfortunately many optical and UV lines are not observable with current technology, as they are invisible against the stellar spectrum. In particular, we predict a luminosity of \( 3.3 \times 10^{-5} \) for the Mg \( i \) line at 4573 \( \AA \), for undepleted Mg abundances. This corresponds to only a few % of the continuum flux level for a photosphere of 4000 K and for an assumed resolving power of 50,000. While this line might be detectable under favorable circumstances where disk gas is not strongly depleted, we are unaware of any such detections in the literature.

The predicted absolute flux of the various lines depends, of course, on the details of the disk structure, the gas abundances, and the ionizing spectrum. As an example, MGN08 show, for a fixed disk structure, the dependence of the predicted flux of a number of fine-structure and forbidden lines on the assumed X-ray luminosity. Furthermore, lines with very low critical densities

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**Table 2**

**Hydrogen Recombination Lines**

| Transition | Wavelength (Å) | Luminosity \((L_\odot)\) |
|------------|----------------|----------------------|
| 2-1......... | 1215.68        | 3.0E-05              |
| 3-2......... | 6564.70        | 2.6E-06              |
| 4-2......... | 4862.74        | 9.5E-07              |
| 4-3......... | 18756.3        | 3.2E-07              |
| 5-2......... | 4341.73        | 4.7E-07              |
| 5-3......... | 12821.7        | 1.6E-07              |
| 5-4......... | 40522.8        | 7.8E-08              |
| 6-2......... | 4102.94        | 2.9E-07              |
| 6-3......... | 10941.2        | 9.8E-08              |
| 6-4......... | 26258.8        | 4.6E-08              |
| 7-2......... | 74598.8        | 2.5E-08              |
| 7-3......... | 3971.24        | 2.0E-07              |
| 7-4......... | 10052.2        | 6.7E-08              |
| 7-5......... | 21661.3        | 3.1E-08              |
| 7-6......... | 46537.9        | 1.6E-08              |
| 8-2......... | 123719         | 9.8E-09              |
| 8-3......... | 3890.19        | 1.5E-07              |
| 8-4......... | 9548.65        | 5.0E-08              |
| 8-5......... | 19450.9        | 2.2E-08              |
| 9-2......... | 37405.7        | 1.2E-08              |
| 9-3......... | 3836.51        | 1.2E-07              |
| 9-4......... | 9211.60        | 4.0E-08              |
| 10-2......... | 18179.2        | 1.7E-08              |
| 10-3......... | 3799.01        | 1.0E-07              |
| 10-4......... | 9017.44        | 3.5E-08              |
| 11-2......... | 17366.9        | 1.4E-08              |
| 11-3......... | 3771.74        | 9.6E-08              |
| 11-4......... | 8865.27        | 2.9E-08              |
| 12-2......... | 16811.2        | 1.2E-08              |
| 12-3......... | 3751.25        | 8.5E-08              |
| 12-4......... | 16411.7        | 1.1E-08              |
| 13-2......... | 3735.47        | 7.7E-08              |
| 13-3......... | 8667.45        | 2.3E-08              |
| 13-4......... | 16113.8        | 1.0E-08              |
| 14-2......... | 3723.03        | 6.8E-08              |
| 14-3......... | 8600.81        | 2.1E-08              |
| 14-4......... | 15884.9        | 9.1E-09              |
| 15-2......... | 3713.06        | 6.1E-08              |
| 15-3......... | 8547.78        | 1.8E-08              |
| 15-4......... | 15705.0        | 8.1E-09              |

Note.—The flux at a distance \( D \), assuming a face-on orientation of the disk, is obtained by dividing the line luminosities by \( 4\pi D^2 \).
such as the C \text{i} and C \text{ii} fine-structure lines (see Table 3) are also very sensitive to conditions in the outer regions of the disk, where densities are small. These regions are preferentially illuminated by the interstellar (or intracluster) radiation fields that are not included in our current simulations.

Unfortunately, Table 1 is not yet complete, as reliable collision strengths were not available for all species, and a number of less abundant elements were omitted from our calculations in order to limit computational costs. In particular, the following species were not included, due to lack of atomic data: Ne \text{i}, Mg \text{iii}, Si \text{i}, S \text{i}, Fe \text{i}, Fe \text{iv}, Fe \text{ix}, Fe \text{xi}, and Fe \text{xxi}. Due to its complexity, the Fe \text{ii} ion was also omitted from the present calculations, but will be included in future models.

A further observational complication lies in the difficulty of separating the emission from the disk, the wind, the accretion funnels, and the photosphere. High-resolution spectroscopy offers one possibility, that in which line profiles that are shifted and/or broadened to different extents in the different emission regimes can be resolved (e.g., Herczeg et al. 2007). Following the suggestion in MGN08, in future work we will present predicted profiles for a number of potentially observable lines emitted from different regions of the disk. An alternative way to distinguish lines formed in the upper layers of the disk and those formed in the accretion funnel would involve comparing transitions with different critical densities (e.g., O \text{i} \lambda 6302 with \text{N}_{\text{crit}} = 1.5 \times 10^9 \text{ cm}^{-3}, compared to O \lambda 63 \mu\text{m} with \text{N}_{\text{crit}} = 2 \times 10^4 \text{ cm}^{-3}).

We note that some of our predicted line intensities differ somewhat from those calculated by MGN08. In most cases, the differences may be explained by the fact that our work used a different disk model for the underlying gas density distribution and different gas abundances. By way of comparison, we have also computed a model that uses the same input parameters and disk model as those of MGN08, and we compare the predicted line fluxes to those of MGN08 in Table 3. Most of the lines listed are in reasonable agreement, particularly when one considers the two different approaches to the problem and the use of different atomic data. MGN08 predict larger \text{[Ne ii]} 12.8 \mu\text{m} line luminosities than in our model; this is explained by the fact that MGN08 do not include cooling by the \text{[Ne ii]} line, which, as already noted by Gorti & Hollenbach (2008), is found to be important. As a consequence, the gas temperature in the \text{[Ne ii]} emitting region will be higher in the calculations of MGN08, producing a larger \text{[Ne ii]} 12.8 \mu\text{m} luminosity. The C \text{ii} fine-structure line at 158 \mu\text{m} shows a larger discrepancy and deserves further attention. Because the critical density of this line is low (see Table 3), it will be collisionally quenched at even modest depths into the disk, and will be preferentially emitted in the less dense upper layers of the disk corona.

MGN08 calculations, however, were focused on the characterization of lower layers in the disk and stopped short of the corona, with the result that some of the flux from the C \text{ii}–bright regions is probably missed.

A detailed comparison of the line luminosities predicted by Gorti & Hollenbach (2008) to those predicted by our models is hindered by the different parameters and approaches employed by the two models. However, we note that the \text{[Ne ii]} 12.8 \mu\text{m} luminosity predicted by our models is a factor of 3.3 lower than that derived by their fiducial model (model A, their Table 4). This can be explained by the fact that our density distribution is determined by the dust temperature structure. Indeed, Gorti & Hollenbach (2008) comment that when they assume a dust-determined temperature structure, they obtain a factor of \sim 4 lower \text{[Ne ii]} line luminosities. We also note that our predicted C \text{i} and C \text{ii} fine-structure lines are higher by a factor of \sim 2 than those given by model A in Gorti & Hollenbach (2008). As discussed above, these lines have low critical densities and are therefore extremely sensitive to the details of the density distribution in the emitting region; furthermore, we use a factor of \sim 3 higher elemental abundance for C. These two factors are probably responsible for the small discrepancy at hand. Gorti & Hollenbach (2008) use highly depleted values for the Si elemental abundance; this is the likely cause of the lower (factor of \sim 10) Si \text{ii} 35 \mu\text{m} line luminosities predicted by their models. Finally, the factor of \sim 3 lower O abundance used in their model is probably one of the causes of the small (factor of \sim 1.5) discrepancy with the O \lambda 63 \mu\text{m} line luminosity.

### 5. DISK DISPERSAL BY PHOTOEVAPORATION

Circumstellar disks are observed around the majority of young stars at \sim 10^6 yr (e.g., Lada & Lada 2003). By ages of \sim 10^7 yr, however, only low-mass debris disks are generally observed (e.g., Manning & Sargent 1997; Wyatt et al. 2003), implying disk lifetime of up to a few \sim 10^6 yr. Indeed, recent observations indicate that about 90% of low-mass stars lose their primordial disks at 5–7 Myr (e.g., Haisch et al. 2001; Hartmann 2005; Hernández et al. 2007a). However, very few observations exist of objects in transition between classical T Tauri stars, which still have disks of a few percent of a solar mass, and weak-lined T Tauri stars, which have dispersed nearly all of their circumstellar disks. For example, Hernández et al. (2007b) reported only a 10% frequency of transitional disk candidates among the disk-bearing low-mass stars in their \textit{Spitzer} observations of the Orion OB1 association. This suggests that the mechanism responsible for the final stages of disk dispersal must operate on relatively short timescales—perhaps as short as \sim 10^5 yr (e.g., Duvert et al. 2000; Andrews & Williams 2007).

Photoevaporative heating from both the central star and external sources has been posited as a viable mechanism able to satisfy the two-timescale nature of the problem. A dramatic illustration of the latter is the apparent photoevaporation of Orion proplyds in the vicinity of OB stars (e.g., Johnstone et al. 1998; Adams et al. 2004; Fatuzzo & Adams 2008). Evidence is also accumulating that disk loss is more rapid in more O star–rich clusters, as judged from observed disk frequencies in low-mass stars (e.g., Albacete Colombo et al. 2007; Guarcello et al. 2007; Mayne et al. 2008). We will return to photoevaporation by external sources of radiation in future work and concentrate here on the effect on the disk of irradiation by the central T Tauri star.

Photoevaporation by ultraviolet (UV) radiation from the central star has been investigated by a number of authors (see Alexander [2008], Dullemond et al. [2007], and Hollenbach et al. [2000] for recent reviews). The original models did not couple
photoevaporation with viscous evolution, resulting in disk dispersal timescales exceeding the observational estimates. Subsequently, the “UV switch” model of Clarke et al. (2001), which coupled photoevaporative mass loss to viscous evolution, was able to reproduce the two-timescale behavior implied by the observations. However, a number of problems still remain, as pointed out in Clarke et al. (2001). In particular, current models require that the Lyman continuum emission from the central star does not derive from accretion, an issue that is currently unclear (ACP04). X-ray ionization and heating of the disk corona provide an attractive alternative engine to drive photoevaporative flows. The fact that weak-lined T Tauri stars, for which accretion has nearly ceased, are known to be brighter in the X-ray than classical T Tauri stars, which are still accreting, suggests that the production of X-rays is not linked to accretion. ACP04 estimated an upper limit to the mass loss driven by X-rays and found it to be at best only comparable to that derived for ultraviolet evaporation. They concluded, therefore, that X-ray heating is unlikely to be the dominant disk dispersal mechanism. ACP04 took into account the effects of X-ray photoionization and heating on the hydrostatic structure of a typical T Tauri circumstellar disk, but were limited by the fact that the radiative transfer problem could not be solved self-consistently in two dimensions.

While our models do not yet iterate over the disk density structure, which would undoubtedly be modified by X-ray irradiation, we do calculate the irradiated thermal structure in two dimensions. It is therefore worthwhile to provide an estimate of the mass-loss rates and dispersal timescales implied by our models. We estimate mass-loss rates by locating, at each radial distance, the base of the photoevaporative flow, defined as the height where the local gas temperature exceeds the escape temperature of the gas, defined as

$$T_{es} = \frac{GM}{c_s^2} r,$$

where $M$ is the stellar mass and $R$ is the radial distance. This height is illustrated as a function of radial distance in Figure 6. The figure shows that, between 8 and 40 AU, the height of the photoevaporating envelope follows a nearly linear increase with radial distance from the star (slope $\sim 0.9$). To a first approximation, the mass-loss rate per unit area can be estimated as

$$\dot{\Sigma}_X = \rho c_s,$$

where $\rho$ and $c_s$ are, respectively, the gas density and the sound speed evaluated at the base of the flow.

The left panel of Figure 7 shows $\Sigma_X$, the mass-loss rate per unit area, and the right panel of Figure 7 shows the mass-loss rate from an infinitely thin annulus as a function of radial distance in the disk. $\Sigma_X$ peaks at approximately 12 AU, near the gravitational radius, $r_g$, for gas with sound speed of $\sim 7$ km s$^{-1}$ ($T \sim 6000$ K). We use the definition of $r_g$ given by Hollenbach et al. (1994), where

$$r_g = \frac{GM}{c_s^2}.$$

The value at the peak is $3.1 \times 10^{-12}$ g s$^{-1}$ cm$^{-2}$; this is about a factor of 10 higher than the estimate of ACP04 ($2.6 \times 10^{-13}$ g s$^{-1}$ cm$^{-2}$) and the value obtained by Hollenbach et al. (1994) for UV photoevaporation ($3.9 \times 10^{-13}$ g s$^{-1}$ cm$^{-2}$). We note that both studies considered the case of a 1 $M_\odot$ star; however, since photoevaporation rates scale only weakly with mass ($\sim M^{0.5}$ for EUV photoevaporation and almost linearly for X-ray photoevaporation), this is not sufficient to explain the order-of-magnitude difference with our rates. As discussed in § 5.1, our model has a number of limitations that may result in uncertainties in the derived photoevaporation rates. Taking into account statistical uncertainties in the calculated temperatures alone, we find that our models are also consistent with peak values as low as $\sim 8 \times 10^{-13}$ g s$^{-1}$ cm$^{-2}$, only a factor of $\sim 4$ higher than previous estimates when corrected for the different stellar masses.

The effects of X-ray photoevaporation are significant only between 8 and 40 AU. There is also a small inner region between 0.03 and 0.16 AU, where, in spite of the large escape temperatures, the intense X-ray field causes the disk to lose mass at a rate of $(3-4) \times 10^{-15}$ g s$^{-1}$ cm$^{-2}$. Given the small area at small radii, this does not contribute significantly to the mass loss. The reason for the mass loss being mainly concentrated between 8 and 40 AU...
is that this region lies far enough from the central star for the escape temperatures to become sufficiently low and not so far that the effects of X-ray irradiation become unimportant. In other words, the steep drop in cape temperatures to become sufficiently low and not so far that this region lies far enough from the central star for the effects of X-ray photoevaporation would not be felt until its viscosity accretion rate, $\dot{M}_{\text{ac}}$, has fallen below $\dot{M}_X$, at which point the disk would empty rapidly within 10–20 AU. Understanding the later evolution of the disk, after the region within 10–20 AU has been emptied, requires us to determine whether the disk beyond 20 AU (1) has to accrete into the 10–20 AU region and then be photoevaporated or (2) is more or less fixed in density profile and then overtaken by the outwardly propagating ring of mass loss. Behavior of type 1 (or 2) results if the mass-loss rate increases (decreases) as the hole size increases. This question will be answered in a following study in which we plan to solve for the density structure and the two-dimensional X-ray transport self-consistently.

Our current calculations give $\dot{M}_X \sim 10^{-8} M_\odot$ yr$^{-1}$, implying that disks with $\dot{M}_{\text{ac}} \leq 10^{-8} M_\odot$ yr$^{-1}$ should disperse rapidly and therefore be seldom observed. However, this disagrees with observations of a considerable number of systems in the 0.5–1 $M_\odot$ range that are reported to have accretion rates lower than $10^{-8} M_\odot$ yr$^{-1}$. Indeed, accretion rates as low as $10^{-9} M_\odot$ yr$^{-1}$ are seen in the $-0.2 < \log M_\star < 0$ mass bin in Figure 8 of Gregory et al. (2006), which, by collecting data from a number of authors, shows the correlation between observed mass accretion rates and stellar mass. This indicates that our predicted $\dot{M}_X \sim 10^{-8} M_\odot$ yr$^{-1}$ is probably too high and may point to a weakness in our model (see discussion in § 5.1).

5.1. Limitations of Our Models

A number of important approximations were used in our models, which may lead to uncertainties in the estimates of the photoevaporation rates. One major caveat of our model, already mentioned in this paper, is that the influence of X-ray photoionization and heating on the disk density structure has been ignored. The high gas temperatures reached in the inner regions of the disk would cause an expansion of the gas in the z-direction, as shown, for example, by ACP04. Indeed, their lower value of mass-loss rate is perhaps caused by a larger attenuation of the X-ray field due to the puffed up inner disk material, which is not accounted for by our models. A hot and inflated inner disk could in fact cause a shadowing effect of the regions at larger radial distances, reducing the effects of X-ray photoevaporation there. The magnitude of this effect can be properly estimated only via the simultaneous solution of the two-dimensional radiative transfer problem and the one-dimensional hydrostatic equilibrium problem in the z-direction, which is the aim of a follow-up paper.

Further uncertainties are introduced by the use of the $\rho_c$, approximation in the calculation of photoevaporation rates. In § 5 we discuss how the base of the photoevaporative envelope is defined as the height where the local gas temperature exceeds the escape temperature of the gas. While this is generally a very good approximation in cases in which the temperature and density vary sharply at the ionization front, as for EUV photoevaporation (e.g., Hollenbach et al. 1994), in the case of X-ray photoevaporation presented here, the distinction between the bound and unbound gas is less clear. In other words, a small error in the determination of temperatures in our models would lead to much larger uncertainties in the density, and hence in the estimated photoevaporation rates.

We conclude that while we have shown that X-rays have the potential to drive an outflow, our derived rates should be treated with caution, and we defer firm conclusions to future work.

6. SUMMARY

We have presented a two-dimensional photoionization and dust radiative transfer calculation of a typical T Tauri protoplanetary disk irradiated by a $1.5 \times 10^7$ K ($kT = 1.36$ keV) X-ray radiation field from the central pre–main-sequence star. A detailed characterization of the temperature structure of the upper disk corona was provided, which uncovered the existence of a layer of highly ionized, hot gas in the inner disk regions. The maximum temperatures reached by the gas in the upper corona were mapped across the radial dimension of the disk, showing peaks exceeding $10^6$ K in the innermost regions. The hotter component of the gas in the inner disk and at radii between ~8 and ~40 AU was shown to be unbound, probably part of a photoevaporative flow. To aid future efforts to observe the hot/warm-gas component of T Tauri disks, we provide a substantial list of predicted emission-line luminosities, many of which should already be detectable with current instrumentation.

The temperature structure of the irradiated disk implies a total mass-loss rate of $\sim 10^{-8} M_\odot$ yr$^{-1}$ and a disk dispersal timescale of a few Myr for a disk mass of 0.027 $M_\odot$, which is the mass of the disk structure model we employed. We discuss the limitations of our model and highlight the need for further calculations that solve the two-dimensional radiative transfer problem simultaneously with the one-dimensional hydrostatic equilibrium of disk structure in the polar direction.

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