# GAS HEATING, CHEMISTRY, AND INFRARED SPECTRA IN INTERMEDIATE-AGED DISKS AROUND LOW MASS STARS

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# RESUMEN

Modelamos la emisión de gas y polvo en discos de edad intermedia (~ 107 años) que se extienden entre 1 - 20 UA alrededor de una estrella de una masa solar. Los modelos tratan de manera auto-consistente el balance térmico y la química, y calculan la estructura vertical de densidad y temperatura del disco gaseoso. Los modelos cubren un rango de masas gaseosas  $10^{-3}$  - 1 M<sub>J</sub> y de polvo  $10^{-7} - 10^{-4}$  M<sub>J</sub>, de manera tal que el polvo es ópticamente delgado a la radiación estelar. Nos enfocamos en las líneas de emisión infrarrojas de una variedad de especies gaseosas como son las líneas rotacionales de H<sub>2</sub>, H<sub>2</sub>O y moléculas de CO, así como en líneas de estructura fina de iones y átomos de carbono, oxígeno, azufre, hierro y silicio, muchas de las cuales son observables con el Telescopio Espacial Spitzer. Encontramos que la línea de [SI] 25.23 µm es la línea de emisión más fuerte en un amplio rango de parámetros estelares y de disco, seguida por la emisión de [SiII] 34.8 µm y [FeII] 26 µm. La línea [FeI] es fuerte cuando las masas gaseosas son altas ( $\geq 0.1 M_J$ ). Las líneas rotacionales de H<sub>2</sub> son más dificiles de detectar, a no ser que las masas gaseosas sean mayores ( $\geq 0.1 M_J$ ). Los modelos aquí presentados serán de gran utilidad en estudios infrarrojos futuros sobre la escala de tiempo de dispersión del gas en un disco capaz de formar planetas, así como prueba de modelos de acrecentamiento para la formación de planetasgigantes.

## ABSTRACT

We model gas and dust emission from intermediate-aged ( $\sim 10^7$  years) disks extending 1–20 AU around a solar mass central star. The models self-consistently treat thermal balance and chemistry, and calculate the vertical density and temperature structure of the gas in a disk. The models cover gas masses  $10^{-3} - 1 M_J$  and dust masses  $10^{-7} - 10^{-4} M_J$ , so that the dust is fairly optically thin to stellar radiation. We focus on infrared emission lines from various gas species such as the rotational lines of H<sub>2</sub>, OH, H<sub>2</sub>O and CO molecules and the fine structure lines of carbon, oxygen, sulfur, iron, and silicon atoms and ions, many of which are observable by the Spitzer Space Telescope. We find that the [SI] 25.23  $\mu$ m line is the strongest emission line for a wide range of disk and stellar parameters, followed by emission from [SiII] 34.8  $\mu$ m and [FeII] 26  $\mu$ m. [FeI] 24  $\mu$ m is strong when gas masses are high ( $\geq 0.1 M_J$ ). Emission from the rotational lines of H<sub>2</sub> is more difficult to detect, unless disk gas masses are substantial ( $\geq 0.1 M_J$ ). The models presented here will be useful in future infrared studies of the timescale for the dispersion of gas in a planet-forming disk, and testing core accretion models of giant planet formation.

# Key Words: INFRARED: STARS — STARS: CIRCUMSTELLAR MATTER — STARS: FORMATION — STARS: PLANETARY SYSTEMS: PROTOPLANETARY DISKS

#### 1. INTRODUCTION

Circumstellar disks evolve from gas-rich structures with 1% of the total mass in dust to disks which are observed to be completely devoid of gas and dominated by emission from dust particles. During this process of evolution, the disk, whose dust is initially very optically thick to stellar photons, becomes optically thin in a few million years (Haisch et al. 2001). We focus in this paper on the epoch 1 Myr  $< t \leq 30$  Myr, during which the disk becomes optically thin in dust opacity, but where significant amounts of gas may persist.

There are a number of reasons why gas during this "intermediate-aged" epoch is important in planet formation and disk evolution. Two competing theories exist for the formation of gas giants. Gaseous Jovian-type planets are believed to form in disks via accretion of gas onto rocky cores of a few earth masses (e.g., Lissauer 1993, Pollack et al. 1996), or by gravitational instability in disks leading to the formation of clumps which subsequently contract to form giant planets (Boss 2003). The presence or absence of gas in intermediate-aged disks can potentially discriminate between these two theories.

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In the gravitational instability scenario, gas giants form quickly and the gas may dissipate more rapidly. Longer gas disk lifetimes ( $\geq 10^{6.5}$  years) facilitate the formation of gas giant planets through conventional core accretion models, allowing sufficient time for the building of a rock/ice core of a few  $M_{\oplus}$ , and subsequent accretion of gas. At this stage of gas accretion, there would be little dust in the gas giant regions of disks, and substantial amounts ( $\gtrsim$  a Jupiter mass,  $M_J$ ) of gas. Core accretion theory suggests that systems may reside in this state for a significant length of time (few Myr, e.g., Pollack et al. 1996). The detection of gas infrared emission lines during this epoch of gas accretion onto rock/ice cores would help support the core accretion scenario. Conversely, if very little gas ( $\ll 1 M_J$ ) is present at the moment when the dust disk first becomes optically thin (signalling the buildup of several earth mass cores), then the core accretion model is likely invalid.

In the terrestrial planet region of the disk, the residual gas content of the disk at the epoch when embryos or protoplanets assemble to form terrestrial planets helps determine the ultimate mass and eccentricity of the planet, and therefore the eventual habitability of the planet (Agnor & Ward 2002, Kominami & Ida 2002). In particular, a narrow range of gas masses produces earth-mass planets on circular orbits. If the gas mass inside 3 AU at ages of  $10^{6.5}$  to  $10^{7.5}$  years is  $\gg 10^{-2}$  M<sub>J</sub>, the tidal interaction of the planets with the gas is sufficient to circularise the orbits of lunar-mass protoplanets, making it difficult for collisions between them to build earthmass planets. On the other hand, if the gas inside 3 AU is  $\ll 10^{-2}$  M<sub>J</sub>, earth-mass planets can be produced, but in orbits considerably more eccentric than that of the Earth.

### 2. THE THERMAL/CHEMICAL MODEL

Disk Overall Properties. Our disk models, described in detail in Gorti & Hollenbach (2004), include chemistry and thermal balance in a selfconsistent manner and calculate the density and temperature structure of the disk in both the radial and vertical directions. The vertical structure of the disk is calculated by balancing the hydrostatic thermal pressure gradient with the vertical component of gravity from the central star. The inner  $(r_i)$  and outer  $(r_o)$  boundaries of the disk and the distribution of the gas and dust surface density  $\Sigma(r)$  within these boundaries are input parameters. In our standard model, we assume  $r_i = 1$  AU,  $r_o = 20$  AU, and  $\Sigma(r) \propto r^{-1}$ .

*Dust Properties.* Coagulation processes in intermediate-aged disks may lead to a distribution

of solid particles which range in size from 1  $\mu$ m to 10<sup>4</sup> km (planets). We define "dust" to consist of all particles  $\leq a_{max} = 1$  mm in radius. We assume that the size distribution of dust particles between  $a_{min}$  and  $a_{max}$  follows a power law  $n(a) \propto a^{-3.5}$  such that most of the surface area is in the smallest particles and most of the mass is in the largest dust particles.

Implicit in these assumptions is that most of the mass of solids will be hidden in objects larger than "dust": e.g., rocks, boulders and planetesimals which emit insignificant amounts of infrared and millimeter wavelength radiation. Thus, at intermediate disk ages (~  $10^7$  years), where solids have grown to planetary sizes but where the gas may not yet have been dispersed, the gas to "dust" mass ratio may increase significantly above the value  $\sim 100$  characteristic of interstellar conditions. Later, as the gas disperses, the gas to dust mass ratio may fall below the interstellar value. In order to express the large range of gas to dust mass ratios and the absolute values of the gas or dust mass which may exist as intermediate-aged and debris disks evolve, we consider a range of gas masses  $M_{gas} \simeq 10^{-3} - 1 \text{ M}_J$  and a range of dust masses  $10^{-7} - 10^{-4} \text{ M}_J$  which are treated as independent variables, so that we cover gas-to-dust mass ratios of  $10^7$  to 10. We emphasize that these masses lie at  $r \leq 20$  AU. We do not consider gas masses smaller than  $10^{-3}$  M<sub>J</sub> because we find such small masses to be undetectable by the Spitzer Space Telescope, SOFIA or Herschel. We do not consider dust masses higher than  $10^{-4}$  M<sub>J</sub> because we find that the dust becomes significantly optically thick in the equatorial plane, and our model is only valid for small to moderate dust optical depths.

Stellar Properties. The stellar spectrum is chosen to be a modified Kurucz model for a G star at 6000 K. The central star at an age  $\sim 1 - 10$  Myr has a significantly higher FUV luminosity than its main-sequence counterpart and we account for this increased luminosity by following a prescription by Kamp & Sammar (2003) for age-dependent FUV fluxes. For the stellar X-ray spectrum we use a fit to ROSAT observations (Feigelson & Montmerle 1999) for a wTTS. For our standard case, the X-ray luminosity is assumed to be  $10^{-4}$  times the bolometric luminosity of the star.

Chemistry. The chemical composition of the gas disk is critical to the structure and evolution of the disk. Although  $H_2$  cooling is often important in the radial range we consider, trace species such as S, O, CO and  $H_2O$  are often significant or even dominant coolants and for an accurate determination of the strength of emission lines, the abundances of atoms



Fig. 1. Gas temperature (solid line) and density (dashed line) as a function of z at a radial position of 2 AU and the temperature at 10 AU for the standard disk model. The dominant heating agents and the coolants in each region are marked on the temperature curve.

and molecules need to be calculated. Our treatment of disk chemistry is an adaptation of the Photodissociation Region (PDR) models of Tielens and Hollenbach (1985) and subsequent work (Kaufman et al 1999). One significant addition is the inclusion of X ray photoionization and photodissociation, as in Maloney et al (1996).

Because the dust is optically thin, stellar and interstellar UV radiation is mainly attenuated in the disk by different gas species in various bands and lines. The gas opacity is very high in some regions of the FUV, shielding molecules and atoms from photodissociation and photoionization. The outer disk is shielded from the stellar photons by the inner disk, and the midplane regions are shielded from the ISRF photons by the upper surface layers. Similarly, the X rays from the star tend to be mostly absorbed in the inner regions and at the disk surface.

Thermal Balance. One of the major innovations of this model is the separate calculation of gas and dust temperatures. Most previous models (with the exception of Kamp & van Zadelhoff 2001) assume that the gas temperature equals the dust temperature. While this is certainly valid in the midplanes or central regions of very optically thick disks, it is not accurate for debris or intermediate-aged disks. Here, the relatively weak thermal coupling between gas and dust, and the different processes which heat and cool the gas and dust, can lead to significant temperature differences. Gas in disks can be heated through many different mechanisms, and we mention three important ones. The heating of dust grains by the stellar radiation field and subsequent collisions with gas molecules transfers kinetic energy to the gas thereby heating it. In regions where the columns through the disk are small enough to allow the penetration of FUV radiation, and  $H_2$  is photodissociated to form atomic hydrogen, the gas heating can be dominated by the heat of formation of  $H_2$ . X-rays from the central star dominate the gas heating at the surface and in the inner disk.

The gas in the disk is mainly cooled through radiative transitions of the different species and, where the gas is warmer than the dust, through gas-grain collisions. We include cooling due to atomic and ionic fine structure and metastable lines and by molecular rotational and vibrational lines, using an escape probability formalism.

#### 3. MODEL RESULTS

Standard Model. The standard model has  $M_{gas} = 10^{-2} \text{ M}_J$  and  $M_{dust} = 10^{-5} \text{ M}_J$ . The gas density in the midplane drops from a value of  $\sim 2 \times 10^{11} \text{ cm}^{-3}$  at 1 AU to a value  $\sim 5 \times 10^8 \text{ cm}^{-3}$  at 20 AU. The radial gas columns at the midplane are therefore of order  $10^{24} \text{ cm}^{-2}$ , sufficient to provide significant gas opacity.

The dust temperature drops from  $\sim 300$  K at 1 AU to about 100 K at 20 AU, or roughly as  $T_{dust} \propto r^{-0.4}$ . The gas temperature in the midplane of the disk is very high ( $T_{gas} \gtrsim 1000$  K) at the very inner edge of the disk, but rapidly drops to  $\sim 300$  K, close to the dust temperature, just outside of 1 AU, due to the exponential attenuation of the UV and X ray heating by the gas opacity in the inner disk. The gas temperature then decreases with radius approximately as  $T_{gas} \propto r^{-0.6}$ . This profile is shallower than the solution for the standard disk models  $(T(r) \propto r^{-3/4})$ , e.g. Adams, Shu & Lada 1988), making our standard disk more "flared" by comparison. The dust temperatures are higher than that of the gas over most of the disk midplane and therefore gas-grain collisions heat the gas here.

Figure 1 shows the variation of gas temperature with height at two different disk radii, 2 and 10 AU, and the gas number density with height at 2 AU, with the dominant heating sources and coolants marked at various heights. In the equatorial region where gas-grain collisions dominate the heating, the density(dashed line in Figure 1) can be seen to decrease rapidly with z (recall that for isothermal disks,

Log L/L<sub>o</sub>

он

он

40

Fig. 2. Mid-infrared spectrum in the 24–40  $\mu$ m wavelength region showing the dust continuum and dominant gas emission lines for the standard disk model, assuming a distance to the disk of 30 pc. A spectral resolving power of 600, the highest available on the Spitzer Space Telescope is assumed.

 $n \propto e^{-z^2/H^2}$ , where H is the scale height), leading to a reduced gas-grain coupling and heating, and causing a drop in temperature with height. Several scale heights above the midplane, the attenuating column to the star drops to sufficiently low values that Xray heating begins to dominate and the gas temperature rapidly rises. The main coolant at the surface is [OI]63 $\mu$ m, which is optically thick at these column densities. The column to the surface decreases with height, and the line becomes more optically thin and more efficient at cooling. This leads to a drop in temperature again in the upper disk atmosphere. Figure 1 also shows the temperature profile at a larger disk radius (10AU), where gas temperatures are much lower.

The chemistry can be summarized as follows. Most H is in H<sub>2</sub> and most C in CO throughout the midplane. The oxygen not in CO is primarily in atomic O, although significant amounts ( $\sim 10^{-8} - 10^{-6}$ ) of OH and H<sub>2</sub>O are obtained. There is enough penetration of Si and Fe ionizing photons that most of the silicon and iron is in Si<sup>+</sup> and Fe<sup>+</sup>. However, the sulfur ionizing photons are attenuated, and in the standard case, most of the midplane sulfur is atomic. Above the midplane, the densities and column densities drop, and the molecules are eventually dissociated at some height, and the atoms with



 $\rm Log~M_{gas}/M_{J}$ 

 $H_{a}(17\mu m)$ 

SI(25.2µm)

H, (28µm

SiII(35.4µm)

Fell(26µm)

ionization potentials below 13.6 eV tend to become singly ionized.

Figure 2 shows a partial spectrum for this standard model disk at a distance of 30 pc, with some dominant lines in the 24–40  $\mu$ m band, superimposed on the dust continuum. The lines shown in the emission spectrum are strong enough to be potentially observable by the Spitzer Space Telescope, or future infrared telescopes, such as SOFIA or Herschel.

The [SI] 25.23  $\mu$ m line stands out as a strong coolant in our disk spectrum and as an important diagnostic of the presence of gas at ~1 AU in disks. The possible detection of gas disks in sulfur is one of our main results, as in many cases this line dominates the spectrum and is stronger than the H<sub>2</sub> lines. Other detectable lines in this figure are the FeII fine structure line at 26.0  $\mu$ m, SiII fine structure line at 34.8  $\mu$ m, and water lines at 33  $\mu$ m and 36  $\mu$ m.

These lines are generally optically thick and would correspondingly diminish in strength with the inclination of the disk, being the strongest for a faceon orientation. H<sub>2</sub>, on the other hand, remains optically thin for the parameter range we present here and is not affected by the orientation angle of the disk. Moreover, it is less dependent on the chemical network and the cosmic abundances assumed and directly traces the gas in the disk. However, the H<sub>2</sub> S(0), S(1) and S(2) lines are often weaker than the other gas emission lines discussed above and are



1.2

hence more difficult to detect.

Parameter Study. We have conducted a parameter survey to explore the probability of gas emission line detection above the dust continuum emission for a range of gas-to-dust mass ratios and mass values which would give us detectable infrared line fluxes. Figure 3 shows the change in IR line luminosities due to variations in gas and dust masses, where we have kept all the parameters of our standard model except the gas and dust masses. Roughly, the Spitzer Space Telescope should detect lines with  $L \gtrsim 10^{-7} (d/30 \text{ pc})^2 \text{ L}_{\odot}$ . Figure 3 shows that for line luminosities  $\gtrsim 5 \times 10^{-8} L_{\odot}$ , the luminosity generally scales with a low power (< 1) of gas mass. This means that for disks at distances  $d \gg 30$  pc, considerably more gas mass is required for detection than if  $L \propto M_{qas}$  is assumed.

Dust collisions dominate the heating in the bulk of the H<sub>2</sub> emitting regions. For disks with very low gas masses, the emission from H<sub>2</sub> decreases sharply because of lower densities in the inner disk which reduce the gas heating by collisions with warm dust and which cause greater photodissociation of H<sub>2</sub>, reducing the total amount of warm ( $\sim 100$  K) H<sub>2</sub> gas in the disk.

The SI, FeII, and SiII emission lines are slightly complicated by chemistry in the disk. For disks of low gas mass ( $\leq 10^{-2} M_J$ ), the main sulfur species in the denser regions near the midplane of the disk is atomic sulfur, and sulfur is photoionized near the surface. Iron and silicon are completely ionized throughout the disk if the gas mass is  $\leq 10^{-2} M_J$ . For these gas masses or below, the emission increases as the gas mass increases and as the dust mass increases. A higher dust mass implies more heating through gas-grain collisions and hence warmer gas. As the gas mass increases to  $0.1 M_J$  or higher, the main sulfur-bearing species near the midplane is  $SO_2$ , as sulfur readily turns molecular at these high densities and gas opacities. Here most of the atomic sulfur is in a layer above the midplane where there is enough penetration of stellar radiation to photodissociate  $SO_2$ , but not sufficient to ionize sulfur. Similarly, chemistry also affects the FeII and SiII lines, as there is substantial amounts of neutral iron and silicon in the denser regions (i.e. near the inner

midplane) of the more massive disks. Therefore the SI, FeII and SiII luminosities decrease with increasing gas mass, as the abundance of these species decreases. The emission from [FeI]24 $\mu$ m, on the other hand, increases rapidly with gas mass due to the increased abundance of warm dense FeI gas.

## 4. CONCLUSION

We find exciting prospects for the detection by the Spitzer Space Telescope, SOFIA or Herschel of infrared line emission from the 0.3 AU to 20 AU regions of intermediate-aged disks. Such measurements will provide an empirical measure of the evolution of gas in disks as they transition from planetforming disks to the older, gas-free, debris disks. The discovery of significant amounts of gas ( $\gtrsim M_J$ ) at the  $t \sim 10^{6.5} - 10^7$  year epoch with optically thin dust could signal the gas accretion phase of gas giant planet formation by the core accretion process. The presence of even small amounts of gas at times  $t \sim 10^{6.5}$  to  $10^{7.5}$  years has important effects on terrestrial planet formation in the 0.3-5 AU region.

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