1 Introduction

1.1 Low mass star formation

The current understanding of the formation of low to intermediate mass stars is outlined by Shu et al. (1987). They identified four stages of star formation (see Figures 1.1 and 1.2). In the first stage the dense, heavily obscured cores of a molecular cloud contract as they slowly lose magnetic and turbulent support. When the density of such a core has passed a critical value, it cannot support itself any longer and gravitational collapse sets in. In this second stage, the core collapses onto its center from the inside out (i.e. the inner parts have collapsed into the center before the outer parts display any significant response). The collapsing material will form a protostar in the center of the core. The core material will continue to fall onto the central star. Most of the material will have sufficient angular momentum to prevent it from falling onto the protostar directly and will gather in a rotating accretion disk around it. Viscous turbulence in the disk (caused by hydrodynamic or magnetohydrodynamic processes) will then ensure further accretion of matter onto the protostar. In this third stage a strong stellar wind set in, driving an outflow of material along the rotational axis of the system. Due to a combination of accretion and an ever widening outflow, the enveloping material is dispersed, leaving only a a newly formed star with a circumstellar disk in the fourth stage. At this stage, a low-mass star with disk is called a T-Tauri system, while intermediate-mass stars are called Herbig Ae/Be systems (depending on the spectral type of the central star).

1.2 Disk evolution and planet formation

1.2.1 Global evolution

Circumstellar disks undergo several changes during their lifetimes, estimated to be $10^6 - 10^7$ years, this is illustrated in Figures 1.1 and 1.2. In the embedded phase (third panel of Figure 1.1, the disk is primarily an accretion disk, transporting material from the envelope to the star. In this stage, the disk is thought to be highly turbulent in order to drive the accretion process, and this turbulence will result in an effective mixing in both the radial and the vertical direction. When the envelope has disappeared due to both accretion and outflows, the accretion

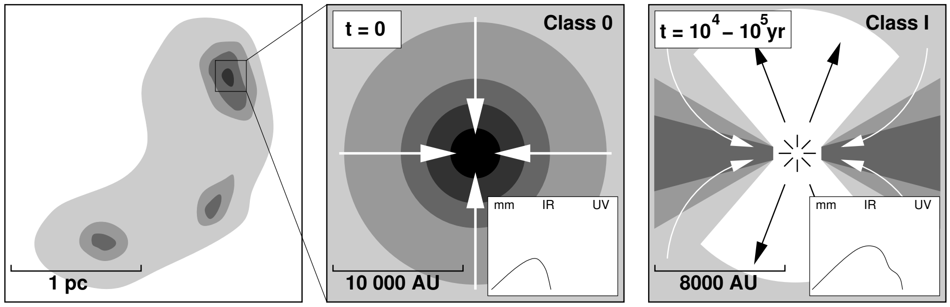

Figure 1.1: Stages 1–3 of low mass star formation according to Shu et al. (1987): slowly contracting dense molecular cores, unstable cores undergoing gravitational collapse, and a protostar collecting material via an active accretion disk surrounded by a remnant envelope. Length scales and timescales since the onset of collapse are indicated in the lower left and upper left corners, respectively. The lower right corner shows a typical SED for the object under consideration.

rate decreases (Hartmann et al. 1998) and a quiescent, passively re-radiating disk remains.

Circumstellar disks are mostly observed around pre-main sequence stars. These disks are relatively massive ($\sim 0.01\ M_\odot$), and most show a flaring geometry (Chiang & Goldreich 1997, see the first panel of Figure 1.2): the scale-height of the disk increases with increasing distance to the central star. As a consequence, the outer parts of the disk intercept a significant fraction of the stellar radiation, and achieve higher temperatures than would be possible in a flat geometry. This causes their spectral energy distributions (SEDs) to be flat at infrared wavelengths, with a sharp cut-off going to millimeter wavelengths.

Some main sequence stars are also found to have disks, but these are much less massive (several $M_\oplus$) than their younger counterparts (see the second panel of Figure 1.2). These objects are called debris disks, since most of the material in these older objects is of second generation origin: the dust particles originate from collisions between planetesimals, while the gas is, at least partly, a product of the evaporation of comets and similar objects. Due to their low masses, the outer parts cannot flare up to intercept stellar radiation, and thus debris disks have a flat geometry. This is reflected in their SEDs, which show a steady shallow decline from infrared to millimeter wavelengths. The disparity in disk masses between stars before and after they have reached the main sequence in the H-R diagram indicates that they undergo a decrease in mass over time. Several processes can contribute to this (for an overview, see Hollenbach et al. 2000): viscous accretion onto the central star, tidal disruption through encounters with nearby stars, strong

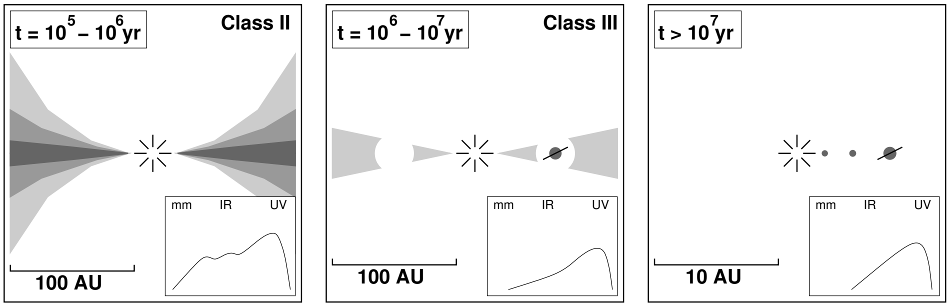

Figure 1.2: As Figure 1.1, but for the final stage of star formation, and the evolution of a circumstellar disk: an optically thick flaring disk, an optically thin debris disk with possible gaps opening due to planet-disk interactions, and a main-sequence star that has dispersed its entire disk where only a planetary system is left.

stellar winds and photoevaporation by the central star or nearby massive stars have been proposed as likely mechanisms. The time scale for disk evaporation is short ($\sim 10^5$ yr) compared to the disk disk lifetime ($\sim 10^7$ yr, Skrutskie et al. 1990), however, and most of the aforementioned mechanisms of disk dispersal cannot account for this. An alternative mechanism was proposed by Clarke et al. (2001): if there is stellar radiation which can ionize atomic hydrogen, this will create a super-hot layer (10^4 K) at the surface of the disk, which can easily escape from the central star's gravity well. Once the rate of evaporation via this route becomes greater than the accretion rate, the disk will quickly evaporate from the inside out.

1.2.2 Dust evolution

While the disk themselves change over time, their contents also show signs of evolution. The most significant of these is the growth of dust particles, detected through the study of disk SEDs at mm wavelengths (Beckwith & Sargent 1991), where the shallow slope of the SED indicates dust grains that are larger than their interstellar counterparts. Another indication that grain growth takes place comes from scattered light imaging (Cotera et al. 2001). In an edge-on disk, the observed width of the dust lane varies for different wavelengths; from this the wavelength dependence of the scattering cross sections is calculated. The wavelength dependence is found to be inconsistent with an interstellar grain size distribution, while it can explained by larger grain sizes. A third indication of grain growth is the observed variation in the $10\,\mu$m solid-state silicate feature (Bouwman et al. 2001). In many disks this feature is broader than in the interstellar medium, which is consis-

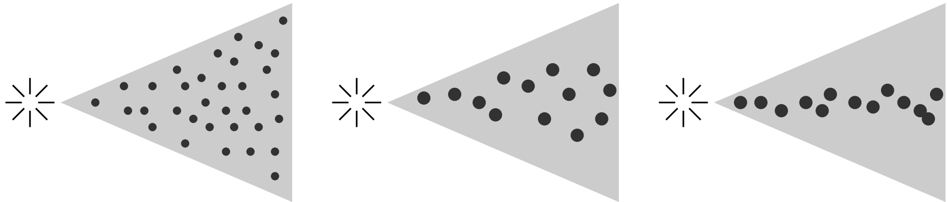

Figure 1.3: Evolution of the dust in disks. In young disks, the interstellar size dust grains are well mixed with the gas. As time goes on, dust grains collide and will stick to each other while drifting slowly downward. The large dust grains will quickly settle in a thin layer in the midplane.

tent with calculations of large grains. Dust grains in circumstellar disks are larger by one or two orders of magnitude than their counterparts in interstellar clouds. It is thought that in the midplanes of disks densities are high enough for initially small dust particles to coagulate, thus forming larger particles (Weidenschilling 1997).

Related to this is the process of dust settling: in disks with sufficiently weak turbulence, the dust grains are not supported by the gas pressure and will drift towards the midplane (see Figure 1.3). Large, heavy dust particles are more susceptible to this effect and will sweep up smaller particles along their way, thus aiding their growth. Dust settling has been detected through examination of disk SEDs (e.g. Miyake & Nakagawa 1995; Furlan et al. 2005). The submillimeter fluxes of some disks are lower than can be explained by a flaring disk, but a flatter disk geometry produces a better fit (cf. the first to panels of Figure 1.2); thus dust settling is likely to have taken place in those disks. Further evidence for dust settling comes from the statistical analysis of observed edge-on disks by D'Alessio et al. (1999). They found a factor 2 less edge-on disks in a sample of 100 than their structure model predicted. Dust settling was put forward as a cause for this discrepancy, since it would decrease the angle from which one would classify a disk as edge-on.

The combined effects of dust growth and settling are considered to be the first step in the formation of planetesimals (Weidenschilling 1997), although current models cannot account for the growth of solid particles beyond cm sizes. Once planetesimals have formed (with sizes of kilometers), their mutual gravity is strong enough to continue planet formation by mutual gravitational attraction (Lissauer 1993). If massive solid bodies form in an early stage of disk evolution they can accrete the surrounding gas, thus forming gaseous giant planets. Another formation mechanism for Jovian planets is through gravitational instabilities in

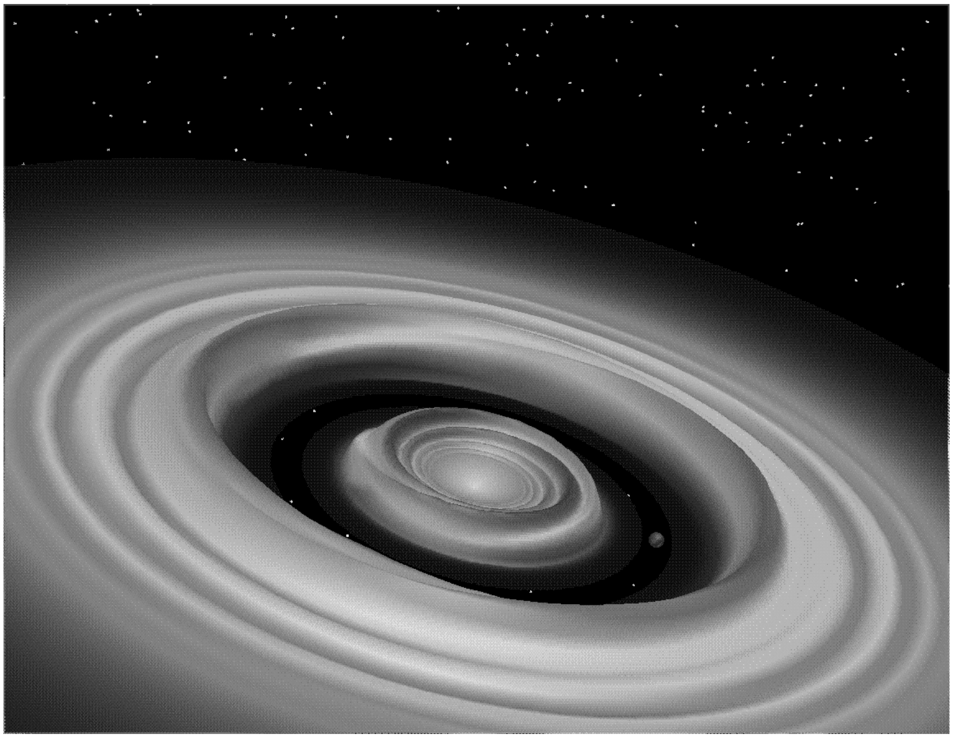

Figure 1.4: Rendering of a hydrodynamical simulation of gap opening in a disk by a giant planet (seen to the right of the central star). The density waves induced by planet-disk interaction are clearly visible.

the gas disk as proposed by Boss (2000). This process requires the disk is self-gravitating, and can therefore only occur if the disk is relatively massive compared to the central star (typically $> 0.1\,M_{\odot}$). When a planet forms, its gravitational influence will cause spiral density waves in the disk and, if the planet is sufficiently massive (typically the mass of Jupiter), sweep up material to open up a gap in the disk (see Figure 1.4). If no gap is formed, the interaction between the planet and the induced spiral waves will cause the planet to migrate (Goldreich & Tremaine 1980), and as a result the planet will quickly fall onto the central star (Tanaka et al. 2002). Planets that open a gap in the disk will undergo inward migration on the longer viscous timescale if the disk is sufficiently massive relative to the planet (Lin & Papaloizou 1986). It remains an open question how the various inward migration processes can be brought to a halt so a planetary system can form.

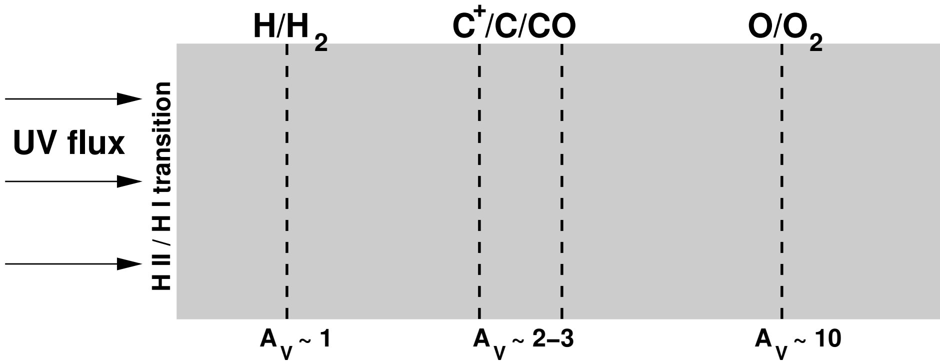

Figure 1.5: Typical structure of a photodissociation region. At the surface all molecules are dissociated by the incident UV flux. With increasing visual extinctions, first hydrogen turns to molecular form, followed by carbon (in the form of CO) and oxygen.

1.3 Photodissociation regions

Photodissociation regions (PDRs; also called photon dominated regions) are the irradiated outer regions of molecular clouds (see Tielens & Hollenbach 1985). They derive their name form the fact that photoprocesses dominate the chemistry and thermal balance. The basic structure of a PDR is shown in Figure 1.5: a gas cloud illuminated on one side by UV radiation. The outer edge of a PDR is traditionally taken as the border between the ionized and neutral gas. Since H_2 is dissociated by line radiation (Solomon, in Field et al. 1966), it can effectively self-shield at relatively low column densities (typically $\sim 10^{14}$ cm^{-2}). Therefore, one goes further into the cloud (at about one magnitude of visual extinction toward the edge), H_2 will become self-shielding, and the gas turns from atomic to molecular. Once hydrogen is mainly in H_2, ion-molecule reactions can proceed to form a variety of molecules Herbst & Klemperer (1973). Temperatures at the surface of a PDR are generally high (100-1000 K) due to the high UV flux which heats the gas via the photoelectric effect. Cooling occurs through the fine-structure lines of O and C^+.

The second most abundant molecule in space, CO, is also subject to self shielding. In general CO becomes completely self-shielding at higher extinctions than H_2, due to the lower cosmic abundances of C and O compared to H (typically a few times 10^{-4}). The dissociative lines of CO partly overlap with those of H_2, causing mutual shielding between these molecules (van Dishoeck & Black 1988). At larger extinctions the UV flux has no noticeable effect on the chemistry any-more, and relatively fragile molecules like O_2 and OH become abundant. With increasing extinction the photoelectric heating decreases, and the gas temperature drops to $\sim$ 10 K. The heating of the gas occurs primarily though cosmic ray ionizations.The chemistry in these regions resembles that of dark clouds, where large organic molecules can form. The low temperatures will cause many molecules to freeze out onto dust grains, enabling surface reactions to further enhance the chemical complexity.

1.4 Disk chemistry

The composition of young disks is expected to be close to that of the molecular cloud they originated in, meaning that the dust grains make up only $\sim$ 1% of the total mass, the remaining 99% being gas. Because of this large difference in mass between dust and gas, the dynamics and evolution of dust grains is tied closely to the gas dynamics. The gas dynamics, on the other hand, are independent of the dust grains. Therefore it is essential to study the gas component of disks in order to understand their behaviour.

The gas in disks can be studied through atomic and molecular lines, either in emission or in absorption against a bright background. The first molecule to be observed in disks was CO (Koerner & Sargent 1995), the second most abundant molecule in interstellar space. Other molecules that have been detected in disks include H_2 (Herczeg et al. 2002), CN, HCN, C_2H, CS, HCO^+ and H_2CO (Dutrey et al. 1997; Thi et al. 2004). The intensities and shapes of these lines depend strongly on the density, gas temperature and chemical structure of the disk.

The density structure can be modeled independently of the gas temperature and chemistry (which are closely interlinked) by calculating vertical hydrostatic equilibrium using the local dust temperature (which can be found by relatively straightforward radiative transfer) to calculate the pressure. The chemistry and gas temperature can be calculated using the density structure found this way (Jonkheid et al. 2004; Kamp & Dullemond 2004), but in recent papers inroads have been made to calculate the densities and gas temperatures iteratively so a self-consistent solution can be found (Gorti & Hollenbach 2004; Nomura & Millar 2005).

There are several processes occurring in disks that influence the chemistry. In the optically thin upper layers, UV radiation from the central star and the interstellar UV field can dissociate and ionize molecules and atoms, and thus these regions resemble dense PDRs. If the central star emits X-rays, they will also have their greatest influence in the surface layers (Gorti & Hollenbach 2004). In the dense and cold regions near the midplane, freeze-out of molecules onto dust grains becomes important, and surface reactions and eventual desorption may take place.

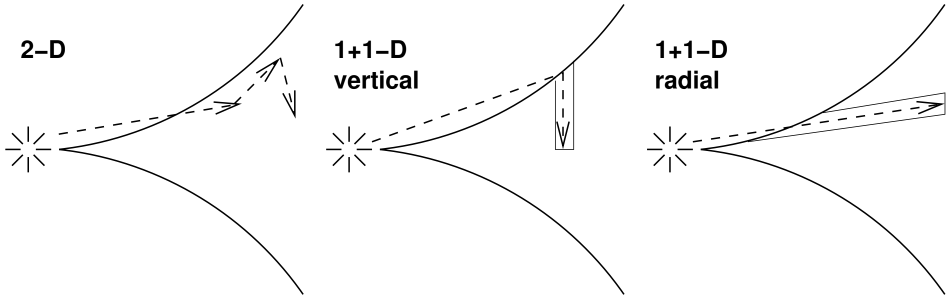

Figure 1.6: Common geometries for UV radiative transfer in disk chemistry models: full 2-dimensional transfer, and 1+1-dimensional transfer with each 1-D structure taken either vertically or radially.

This leads to a three-layered chemical structure (Aikawa et al. 2002; van Zadelhoff et al. 2003): an atomic surface layer where most molecules are dissociated by UV radiation; an intermediate molecular layer where the UV flux is sufficiently low that molecules can survive; and an icy region near the midplane where the temperatures are so low that most molecules freeze out onto dust grains.

The gas temperature in the dense regions near the midplane is equal to the dust temperature. The densities are so high that gas molecules collide often with dust grains and their temperatures equilibrate. Higher in the disk the densities are not high enough for this to occur, an the gas temperature is determined by a balance between heating and cooling processes. Heating of the gas occurs primarily through photoelectric emission of dust grains and polycyclic aromatic hydrocarbons (PAHs); the energetic electrons liberated by this process deliver their energy to the gas. other heating processes that can become important are C photoionization, collisional deexcitation of H_2 and cosmic ray ionization. The gas is cooled through atomic and molecular line emission, most importantly the [C II] and [O I] fine structure lines and the rotational lines of CO. In very hot layers near the surface, the [O I] 6300 Å and Lyα lines can become important. This results in gas temperatures that are significantly higher than the dust temperatures (several 100 K) in the surface regions of the disk. In the regions where the disk becomes optically thick to UV radiation, the gas temperature drops until gas and dust are in thermal equilibrium.

Since UV radiation is so important for the chemistry in the upper layers of the disk, the radiative transfer of stellar and interstellar UV is critical to models of disk chemistry. Ideally, all radiative transfer is done in three dimensions, and due to the intrinsic cylindrical symmetry of disks this can be reduced to effectively two dimensions (van Zadelhoff et al. 2003, see also Figure 1.6). A 2-

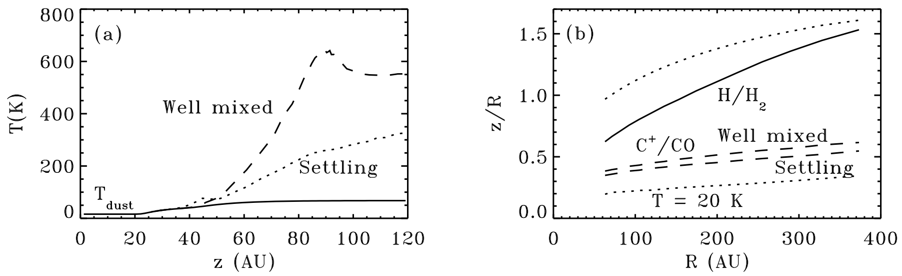

Figure 1.7: Main results from Chapter 3. Panel (a): vertical distribution at R = 100 AU of the dust temperature (solid line) and the gas temperatures for a well-mixed disk (dashed line) and a disk undergoing dust settling (dotted line). Panel (b): 2-dimensional overview of the disk chemistry. The upper dotted line indicates the disk surface; the solid line indicates the H/H_2 transition; the dashed lines indicate the C^+/CO transition; and the lower dotted line indicates the T_{dust} = 20 K isotherm, where CO freezes out on dust grains.

dimensional treatment of the radiative transfer is time-consuming, however, especially if one takes into account the feedback with chemical calculations to get correct results for self-shielding processes. It is therefore often more practical to divide the 2-dimensional grid into a series of 1-dimensional structures (making it a so-called 1+1-dimensional model), since 1-dimensional radiative transfer is relatively straightforward. making a 1+1-dimensional grid can be done in two ways (see Figure 1.6): a number of vertical structures can be stacked in the radial direction, or a number of radial structures can be stacked in the vertical direction. The former is applicable to optically thick disks, in which scattering plays an important role. The latter is applicable in optically thin disks, where scattering will be far less important, and the adopted geometry will simulate radiation traveling in straight lines from the central star.

1.5 Outline of the thesis

The main question addressed in this thesis is how calculations of the chemistry and gas temperature can be used to probe different physical conditions in circumstellar disks. For this purpose the Leiden PDR code was changed so it could be used for 1+1-dimensional and quasi 2-dimensional disk models (see Figure 1.6). The code then calculates the equilibrium values of the gas temperature and the chemical abundances. With the output of the PDR code the line emission of the disk was calculated with the accelerated Monte Carlo line radiative transfer code RATRAN by Hogerheijde & van der Tak (2000). By using different input models, the effects of dust settling, mass loss and gap opening on the gas temperatures, chemistry and emission lines were studied.

Chapter 2 of this thesis is concerned with testing the PDR code used in the other chapters. A benchmark test was done to compare the results of various PDR codes for a number of fixed input values. Special attention was given to the gas temperature solutions given by two participating codes. It was found that the different PDR codes give similar results in the chemistry for several benchmark models after an intensive workshop meeting. Where differences still occur, most notably in the gas temperatures, they can be understood by a close examination of the processes included and the assumptions made in each code.

In Chapter 3 a model is presented in which the chemistry and gas temperature are calculated in a T-Tauri disk, using the density profile and dust temperatures by D'Alessio et al. (1998). The model divides the disk in a number of vertical 1-dimensional PDRs, and treats radiative transfer only in this direction. The calculations were also done for a model where dust particles were largely removed from the surface layers, thus simulating dust settling. It was found that the gas temperature is significantly higher than the dust temperature in the optically thin surface layers of the disk; in the optically thick layers near the midplane the gas temperature becomes equal to the dust temperature. Dust settling was found to have little effect on the chemistry if PAHs are still well mixed with the gas; the C^+/C/CO and the O/O_2 transitions occur only slightly lower in the disk (see Figure 1.7). Dust settling does affect the gas temperature in the upper layers, since the removal of dust grains there directly decreases the photoelectric heating rate. This difference in temperature is reflected in the [O I] fine structure lines, which are sensitive to the high gas temperatures found here.

In Chapter 4 a model of the transitional disk around HD 141569 is presented. This disk is optically thin for continuum radiation, and therefore the PDR structures were calculated in the radial direction rather than vertically. From the chemical model the CO line intensities were calculated and compared to observations to constrain the mass and distribution of the gas in the disk. The models indicate that a 80 $M_\oplus$ disk with a gas distribution between 80 and 500 AU provides a good fit to the observations of CO lines. This means that there is a significant amount of gas present within the inner hole in the dust distribution, which has a radius of 150 AU.

In Chapter 5 the chemistry is calculated in a series of input models that simulate disk dispersal and dust settling in disks around Herbig Ae stars. UV radiative transfer was performed in a fully 2-D fashion in this chapter; the cooling radiation was still treated 1-D in the vertical direction, similar to the model in Chapter 3. For all models molecular emission lines were calculated to find suitable tracers to distinguish between disks where dust is settling and dissipating disks. The gas temperatures in the surface layers of disks with an interstellar gas/dust ratio were found to be even higher than for T-Tauri disks ($> 1000\,K$). The gas temperatures show a steady decrease in the models where dust settling is simulated due to the decreasing photoelectric heating. The chemical structure shows the greatest variation in disks where material is dispersed; the decrease of both the dust extinction and the densities lower the molecular abundances significantly. In disks where dust settling takes place only the extinction decreases while the densities stay constant, and thus the effect on molecular abundances is less pronounced. The shape of the radiation field was found to have a profound effect on the abundances of observable molecules like CN, HCN and C_2H. From the the results of the chemistry line intensities were calculated, and CO/^{13}CO, ^{13}CO/HCO^+ and [O I] 63 μm/146 μm are found to be good tracers to distinguish between overall disk dispersal and dust settling.

1.6 Main results of this thesis

- The gas temperatures in the optically thin surface layers of flaring disks were found to be greater than the dust temperatures; in the optically thick midplane, the two temperatures are equal. The high gas temperatures influence the chemistry by allowing reactions with an activation barrier of several 100 to 1000 K, leading to greater abundances of molecules like CH^+, CO and HCO^+. The high temperatures also affect high-energy emission lines, such as the [O I] fine-structure lines and the high-J CO lines.

- The main effect of dust settling on a disk is a decrease in the gas temperature, as the photoelectric heating is removed. The chemistry shows only limited variation, even when the dust/gas ratio decreases by a factor of 100; the main effect is that the peak in the vertical abundance distribution is shifted slightly toward the midplane. This is mostly due to self-shielding effects, which can shield molecules from UV radiation even in the absence of dust.

- PAHs are found to be very important in the chemistry and thermal balance of disks. If PAHs are present with interstellar abundances, they contribute enough to the heating, extinction and H_2 formation that the effects of dust settling become negligible. Apart from H_2 formation, PAHs also contribute to the formation of CO by allowing such reactions as $\mathrm{PAH:H} + \mathrm{C}^+ \rightarrow$

PAH + CH^+, which can further react to CO^+, HCO^+ and ultimately CO. If PAHs are removed from the disk, the CO abundance will decrease.

- In low-mass disks, CO rotational lines form an excellent tracer of the gas mass. Due to feedback effects of the chemistry on CO self-shielding, there is a domain where the CO abundances depend very strongly on the gas mass. For higher disk masses the dependence disappears, as CO is completely self-shielding and the rotational lines are optically thick.

- The radiation field of a 10 000 K A star results in a chemical structure that is very different from a conventional PDR chemistry. Molecules with dissociation cross sections at $\lambda > 1200$ Å have far larger dissociation rates than molecules that can only be dissociated at shorter wavelengths, due to a discontinuity in the stellar spectrum. This results in large regions of moderate extinction where atomic C is the dominant form of carbon, since CO precursors like CH are easily dissociated; HCN and C_2H have lower abundances than one would expect from PDR models using the flatter interstellar UV spectrum.

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