Modeling Molecular-Line Emission from Circumstellar Disks

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1 Introduction

Most young stars are surrounded by accretion disks [1], which are likely progenitors of planetary systems. The study of the physical structure, chemical composition, and evolution of these disks is therefore clearly a topic of great interest. The thermal emission of dust grains in disks has provided a wealth of information on the disks’ properties. At near-infrared wavelengths, the thermal emission is dominated by a small amount (∼10⁻⁵ M⊕) of warm material close to the star, and the emission is often optically thick. These wavelengths serve as excellent probes of the presence or absence of a disk. At the longer (sub) millimeter wavelengths, the emission probes the cold material at larger radii (>1 AU), where the emission is usually mostly optically thin. These wavelengths are good probes of the total mass of a disk.

Dust, however, only makes up 1% of the total mass of the disk, if we adopt the standard interstellar gas-to-dust mass ratio. Ignoring the difficult to observe H₂ molecule (but see, e.g., [2, 3]), circumstellar disks are now commonly observed through lines of molecules such as CO, HCO⁺, HCN, CN, etcetera. Although it is found that the molecular abundances are often strongly depleted through freezing out onto dust grains [2] and the lines correspondingly weaker, molecular-line observations offer a powerful array of diagnostics to study disks: from the relative intensities of transitions, the molecular excitation can be derived and the density and temperature of the gas constrained; from the line strengths, the molecular abundances are found and the chemical composition inferred; and from the resolved line profiles, the velocity field in the disk is directly probed. This contribution discusses the methods with which this wealth of information can be extracted from molecular lines, and presents examples of recent research that illustrates this.

2 The Physical and Chemical Structure of Disks

Within the framework of standard accretion disks [4, 5], recent theoretical models specifically address their vertical structure [6, 7]. In a system where the central object dominates the mass and the luminosity, the disk is expected to assume a flared configuration, where the hydrostatic scale height increases
with radius $R$. This flared surface intercepts more stellar light, which raises the temperature of the surface and, through reprocessing, of the disk interior (e.g., [2]). Refinements to these models include the effects of dust sublimation and self-shadowing of the outer disk by inner, flared regions [10, 11, 12, 13].

The resulting descriptions of the density and temperature as function of radius and height then serve as input to calculate the abundances of various molecules (e.g., [14, 15, 16, 17, 18, 19, 20, 21, 22, 23]; and Henning, this volume). Three processes affect the molecular gas-phase abundances (reviewed in [24]): (1) freeze-out of molecules onto dust grains in the dense and cold midplane, reducing the gas-phase abundances; (2) evaporation of these ice mantles at intermediate vertical heights and near the star, where the temperatures exceed the evaporation values ($\sim 22$ K for CO, $\sim 90$ K for $\text{H}_2\text{O}$) and where species return to the gas; and (3) dissociation and ionisation by (inter-) stellar ultraviolet photons in the disk surface where there is insufficient shielding by dust, $\text{H}_2$, and CO, and where a chemistry akin to a photon-dominated region is set up (see Sternberg, this volume). Radial inflow and vertical convection further influence the disk’s chemical structure.

3 Radiative Transfer and Molecular Excitation

With a model in hand for the physical and chemical structure of the disk (density, temperature, systematic and turbulent velocity fields, and gas-phase abundances – all as functions of radius $R$ and height $z$), the emergent emission (or absorption) lines can be calculated. An iterative approach is usually chosen: Starting with an educated guess for the level populations throughout the disk (or at a sufficient number of grid points), the absorption and emission coefficients are evaluated and the radiative transfer through the disk is solved (along a sufficient number of photon paths). This yields the intensity of the radiation field throughout the disk, with which the equations of statistical equilibrium can be solved and an update to the level populations found. This procedure is repeated until the solution converges.

Several factors complicate this prescription in circumstellar disks. Disks have a large range in density and temperature, with molecular excitation ranging from thermodynamic equilibrium to sub-thermal. Molecular abundances can vary by several orders of magnitude within the disk. Opacities, both in continuum and in lines, can be large. These factors require that the input model contains sufficient detail to cover the variations in excitation and abundance, and necessitate careful assessment of the convergence of the solution: large opacities can strongly slow down the convergence, because at each iteration step, changes in the population only propagate over short distances (corresponding to $\tau \sim 1$).

Increased computer speed and memory has made realistic model calculations tractable. In 1999 in a workshop at the Lorentz Centre in Leiden, several of the leading codes for molecular excitation and radiative transfer
were (successfully!) tested against each other\(^1\). The reliability of the obtained solutions depends on the quality of the molecular collision rates that are used; several projects are under way to provide accurate rates for astrophysically relevant species (see Roueff, this volume; and Schöier et al. in prep.\(^2\)).

Slow convergence of iterative methods in the presence of large opacities is not only an inconvenience for the impatient, but may lead to incorrect results. Convergence is often judged on the difference between subsequent iterations, with the implicit assumption that this will be small only when the solution is close to the correct value. The small differences between subsequent solutions due to opacity is easily misinterpreted as convergence. In the modeling of stellar atmospheres these problems are well understood, and have lead to the development of acceleration techniques such as Accelerated Lambda Iteration \(^25\) (ALI; Lambda Iteration refers to iterative solution methods). Acceleration techniques have been included in Monte Carlo approaches to solve the radiative transfer \(^26\). This combines the reliability of accelerated convergence with flexibility in addressing arbitrary geometries.

4 Examples

**Resolved Disk Emission of LkCa 15.** Using the millimeter array of the Owens Valley Radio Observatory (OVRO), the emission of the 450 AU radius, 0.18 \(M_\odot\) disk around the young star LkCa 15 has been resolved \(^27\) \(^28\). \(^{12}\)CO \(J=2\rightarrow1\) emission peaks at the source, with velocities consistent with Keplerian rotation of an inclined \((i \approx 60^\circ)\) disk around a 0.8 \(M_\odot\) star. In stark contrast, the emission of CN \(1\rightarrow0\) and HCN \(1\rightarrow0\) is broken up in two peaks, symmetrically displaced from the star by \(\sim 2'' \approx 300 \text{ AU}\).

The appearance of HCN and CN can be reproduced by a simple radial ‘step function’ for the abundance, with CN and HCN only present outside 300 AU \(^29\). This can be explained by chemistry in a flared disk, where only outside \(\sim 300 \text{ AU}\) densities are low enough to allow ultraviolet radiation to penetrate and set up a PDR with increased abundances of HCN and CN. Self-consistent calculations are currently under way (Kessler et al., in prep.).

**Two-dimensional Transport of Ultraviolet Radiation.** To accurately account for the penetration of ultraviolet radiation from the central star into the flared disk, the full details of the two-dimensional transfer must be included \(^30\). Compared to one-dimensional calculations that only include vertical transport, the predominantly forward-scattering nature of the grains causes the ultraviolet field to penetrate deeper. A larger fraction of the disk is subject to photo-chemistry, with increased abundances of radicals like CN and \(C_2H\).

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\(^1\) For more information, see [http://www.strw.leidenuniv.nl/~radtrans](http://www.strw.leidenuniv.nl/~radtrans).

\(^2\) Available through [http://www.strw.leidenuniv.nl/~moldata](http://www.strw.leidenuniv.nl/~moldata) and [http://basecol.obs-besancon.fr](http://basecol.obs-besancon.fr).

\(^3\) Available at [http://www.strw.leidenuniv.nl/~michiel/ratran.html](http://www.strw.leidenuniv.nl/~michiel/ratran.html).
An interesting application is the effect of the accretion-generated ultraviolet radiation field on the HCN and CN chemistry. Two-dimensional calculations show that the CN/HCN abundance ratio increases by a factor of 10 if an ultraviolet excess similar to that of TW Hya is included on top of a 4000 K stellar blackbody. The ratio of the CN 3–2 line emission over HCN 4–3 increases by a similar amount, albeit confined to a region from the star at a typical distance of 140 pc for the object. Instruments like the Smithsonian Submillimeter Array (SMA) and the Atacama Large Millimeter Array (ALMA) will be able to trace such regions.

Far-infrared $^{12}$CO Line Emission from Superheated Disk Surfaces. The object Elias 29 is a T Tauri star with a face-on disk of 0.012 M$_\odot$ that is obscured behind several layers of interstellar clouds. It shows $^{13}$CO 6–5 and $^{12}$CO lines up to at least 20–19, indicating the presence of ~ 0.001 M$_\odot$ of warm (> 200 K) gas. This reservoir of warm gas may be explained by material heated in outflow shocks, but is also comparable to the amount of material expected in the superheated surface layer of the flared disk around Elias 29.

Standard flared disk models cannot produce sufficient far-infrared $^{12}$CO line emission: although the amount of warm gas is sufficient, its density is too low to excite these lines. In the standard flared-disk model, perfect mixing between gas and dust is assumed. If, however, the grains have settled toward the midplane, the superheated layer extends further into the denser disk interior. Calculations indicate that $^{12}$CO far-infrared line strengths in this case can even exceed the observed values. Although more detailed modeling is required, including the fate of small dust grains that will not decouple from the gas, this scenario suggests that the superheated layer is a viable source of far-infrared CO emission.

Rotation and Infall in the Disk Around L1489 IRS. Submillimeter-continuum and millimeter aperture-synthesis observations show that the object L1489 IRS is surrounded by a flattened structure of ~ 2000 AU radius and ~ 0.02 M$_\odot$ mass. While this mass is entirely typical for disks around T Tauri stars, its size exceeds by a factor of 2–3 the largest known gas disks. Through modeling of the HCO$^+$ 1–0 and 3–2 interferometer images, the velocity field in the disk can be obtained. In addition to a Keplerian component, suggesting a central mass of 0.65 M$_\odot$, inward motions amounting to ~ 10% of the total velocity vector are found. If such motions continue inward to the star (the interferometer data only sample scales > 700 AU), the disk lifetime is ~ $2 \times 10^4$ yr. This is much shorter than the estimated duration of the embedded (few times 10$^5$ yr) and T Tauri (few times 10$^6$ yr) phases. It suggests that L1489 IRS represents a short-lived transitional stage, where the collapsing cloud core is settling onto a rotationally supported disk.

The inward motions can be followed to within 0.1 AU from the star through $^{12}$CO fundamental ro-vibrational absorption lines against the stellar
continuum at 4.7 \( \mu m \) \[35\]. The line profiles of the individual components of the P- and R- branches show prominent wings extending to +100 km s\(^{-1}\). Such velocities are expected to occur within 0.1 AU from the star, based on the velocity model derived from the HCO\(^+\) measurements above. The presence of absorption line originating from rotational levels of \( J=6 \) and above indicate temperature exceeding 100–200 K, which also are only expected to be populated close to the star. Taken together, this shows that the inward motions are present from 2000 AU as traced by the HCO\(^+\) data to within 0.1 AU probed by the CO absorption.

There are several objections against the interpretation that the entire disk around L1489 IRS is contracting. The implied mass accretion rate exceeds observational limits \[36\] by more than an order of magnitude. And the theoretical models for accretion flow predict subsonic motions, while the observed speeds are supersonic. A possible solution is that only a thin, unstable surface layer participates in the inflow, while the bulk of the disk is Keplerian. Another solution posits the existence of two regions of inflow: one at large radii (probed by the HCO\(^+\) data) where the cloud’s material spirals onto the outer disk, and one at small radii (probed by the CO line wings) where material streams from the disk onto the star. The fact that both regions can be fit with the same velocity model does not require them to be physically connected, because the motions occur in the gravitational potential of the same star. Further study of the L1489 IRS aims at distinguishing these scenarios (Hogerheijde et al., in preparation).

5 Conclusion

In this contribution I have shown that there now exist increasingly realistic two-dimensional and three-dimensional models of the physical and chemical structure of disks. Radiative transfer and molecular excitation tools have been developed that can calculate the emergent line spectrum on the basis of these disks models. On the observational side, current data are beginning to probe the structure of disks, although with no more than a few resolution elements across the objects. The first results show interesting structural differences between various probe molecules, which current chemical models can explain.

In the next few years, increasing detail is to be expected in disk models, as the increased speed of computers will bring more extensive modeling within reach. With the arrival of new observational facilities in the submillimeter (SMA, CARMA, ALMA) and the infrared (SIRTF, SOFIA, Herschel), molecular-line modeling will form an essential link in comparing models with data. By the end of this decade, our understanding of protoplanetary disks will likely have progressed significantly.

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References

1. S. V. W. Beckwith and A. I. Sargent: Nature 383, 139 (1996)
2. W. F. Thi, E. F. van Dishoeck, G. A. Blake, G. J. van Zadelhoff, J. Horn, E. E. Becklin, V. Mannings, A. I. Sargent, M. E. van den Ancker, A. Natta, and J. Kessler: ApJ 561, 1074 (2001)
3. M. J. Richter, D. T. Jaffe, G. A. Blake, and J. H. Lacy: ApJL 572, L161 (2002)
4. D. Lynden-Bell and J.E. Pringle: MNRAS 168, 603 (1974)
5. J. E. Pringle: ARA&A 19, 137 (1981)
6. P. D’Alessio, J. Canto, N. Calvet, and S. Lizano: ApJ 500, 411 (1998)
7. E. I. Chiang and P. Goldreich: ApJ 490, 368 (1997)
8. N. I. Shakura and R. A. Sunyaev: A&A 24, 337 (1973)
9. S. J. Kenyon and L. Hartmann: ApJ 323, 714 (1987)
10. C. P. Dullemond: A&A 361, L17 (2000)
11. C. P. Dullemond, C. Dominik, and A. Natta: ApJ 560, 957 (2001)
12. C. P. Dullemond, G. J. van Zadelhoff, and A. Natta: A&A 389, 464 (2002)
13. C. P. Dullemond and A. Natta: A&A 405, 597 (2003)
14. Y. Aikawa, S. M. Miyama, T. Nakano, and T. Umebayashi: ApJ 467, 684 (1996)
15. Y. Aikawa, T. Umebayashi, T. Nakano, and S. M. Miyama: ApJL 486, L51 (1997)
16. Y. Aikawa, T. Umebayashi, T. Nakano, and S. M. Miyama: ApJ 519, 705 (1999)
17. Y. Aikawa and E. Herbst: A&A 351, 233 (1999)
18. Y. Aikawa and E. Herbst: ApJ 526, 314 (1999)
19. Y. Aikawa and E. Herbst: A&A 371, 1107 (2001)
20. Y. Aikawa, G. J. van Zadelhoff, E. F. van Dishoeck, and E. Herbst: A&A 386, 622 (2002)
21. K. Willacy and W. D. Langer: ApJ 544, 903 (2000)
22. A. J. Markwick, M. Ilgner, T. J. Millar, and T. Henning: A&A 385, 632 (2002)
23. E. Bergin, N. Calvet, P. D’Alessio, and G. J. Herczeg: ApJL 591, L159 (2003)
24. E. F. van Dishoeck and G. A. Blake: ARA&A 36, 317 (1998)
25. G. B. Rybicki and D. G. Hummer: A&A 262, 209 (1992)
26. M. R. Hogerheijde and F. F. S. van der Tak: A&A 362, 697 (2000)
27. C. Qi: Ph.D. Thesis, Calif. Inst. of Tech., Pasadena (2001)
28. G. Duvert, S. Guilloteau, F. Ménard, M. Simon, and A. Dutrey: A&A 355, 165 (2000)
29. J. E. Kessler, G. A. Blake, C. Qi, and J. Brown: BAAS 34, 1319 (2002)
30. G.-J. van Zadelhoff, Y. Aikawa, M. R. Hogerheijde, and E. F. van Dishoeck: A&A 397, 789 (2003)
31. A. C. A. Boogert, M. R. Hogerheijde, C. Ceccarelli, A. G. G. M. Tielens, E. F. van Dishoeck, G. A. Blake, W. B. Latter, and F. Motte: ApJ 570, 708 (2002)
32. C. Ceccarelli, A. C. A. Boogert, A. G. G. M. Tielens, E. Caux, M. R. Hogerheijde, and B. Parise: A&A 395, 863 (2002)
33. M. R. Hogerheijde: ApJ 553, 618 (2001)
34. M. R. Hogerheijde and G. Sandell: ApJ 534, 880 2000.
35. A. C. A. Boogert, M. R. Hogerheijde, and G. A. Blake: ApJ 568, 761 (2002)
36. J. Muzerolle, L. Hartmann, and N. Calvet: AJ 116, 2965 (1998)