Molecular gas and dust influenced by massive protostars
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Summary and future directions

ABSTRACT

In this thesis, I have studied the effects that massive protostars have on surrounding dust and molecular gas. High-mass protostars \((\gtrsim 8 \, M_\odot)\) are distinct from their lower mass counterparts, because they require higher mass accretion rates, produce orders of magnitude more energy and emit this mainly at UV wavelengths. This radiation impedes mass accretion and alters the chemical composition of the circumstellar material (see chapter 1).

This final chapter summarizes the main conclusions of each preceding chapter in this thesis. I also take this opportunity to describe possible future directions of research related to each subtopic.
7.1 Star formation in dark clouds

(Chapter 2)

The story of this thesis starts in chapter 2 with an investigation of a so-called InfraRed Dark Cloud (IRDC). IRDCs, condensed regions of the ISM with column densities \( \gtrsim 10^{23} \text{ cm}^{-2} \) and temperatures below 25 K, are suspected sites of high-mass star formation. I analyze Spitzer Space Telescope multiband photometry of one such IRDC, G048.65−00.29, at a distance of 2.5 kpc, in a field that spans several parsecs in length scale. In these observations, individual young stellar objects (YSOs) are not spatially resolved, but the total field of view allows to obtain an overview of several associated protostellar candidates.

The 24 \( \mu \text{m} \) MIPS band reveals twenty point sources. Fourteen of these sources are identified as young stellar objects, using counterparts in the shorter wavelength IRAC bands, as well as near-infrared 2MASS measurements and submillimeter datapoints from the literature. Similar to what is seen in far-infrared Herschel maps of the Aquila rift region (André et al. 2010), the YSOs in our field are distributed primarily along the filamentary shaped dark cloud. The method employed to identify and characterize the YSOs is a fit of the observed datapoints to the grid of modeled spectral energy distributions for YSOs by Robitaille et al. (2006, 2007). I find that stellar masses of the YSOs range from slightly sub-solar to \( \sim 8 M_\odot \), which implies that this IRDC only hosts low- to intermediate-mass YSOs. Although the selection of 24 \( \mu \text{m} \) sources probably covers the youngest and most massive objects (chapter 2.4.2), further exploitation of this dataset is likely to identify additional YSOs detected only in IRAC bands. Moreover, I find YSOs in various evolutionary stages, indicating that the star formation in this cloud is not an instantaneous process.

The finding that IRDC G048.65−00.29 hosts no massive protostars is in contrast with the popular view of IRDCs as sites of high-mass star formation. The object studied in chapter 2 may be special in that sense, or future studies may find more IRDCs with only relatively low-mass star formation activity associated to them. Therefore, statistical studies of YSO populations in other IRDCs will have to confirm or disprove the one-to-one relationship of massive young stars and IRDCs. Such studies are facilitated by publicly available infrared surveys of the Galactic plane, such as UKIDSS, GLIMPSE and MIPSGAL (Lawrence et al. 2007; Benjamin et al. 2003; Carey et al. 2006), and IRDC catalogs by Simon et al. (2006a) and Peretto & Fuller (2009). The catalog of IRDC-like objects in the outer Galaxy by Frieswijk & Shipman (2010) provides a starting point for investigations of the star formation process under different metallicity conditions. With the Herschel Hi-GAL survey (Molinari et al. 2010a,b), work is ongoing to bridge the gap between the submillimeter and mid-infrared photometric surveys. Further knowledge should be added to the existing infrared legacy by the Japanese-European SPICA mission around the year 2020. These observational advances will provide a more complete picture of objects
in their earliest evolutionary stages and provide an opportunity to answer questions like: do dark clouds exist that stay dark beyond the mid-infrared?

Finally, the variety of options for continuum studies of YSOs associated to IRDC structures is complemented by the potential of specific molecular line tracers. For example, unpublished JCMT A-band spectra show outflow wings in optically thick CO lines toward the brightest 24 μm and submillimeter source in G48. At the same time, the well-known shock tracer SiO is not detected in its 5–4 transition, with an upper limit to the peak intensity of ~1% of the detected C^{18}O 2–1. In addition, ongoing Herschel/HIFI studies of H_{2}O lines in a selection of other IRDCs show complex, self-absorbed line profiles, indicative of outflow activity in relatively early evolutionary phases (Shipman, Van der Tak, Frieswijk et al. 2011, in preparation).

### 7.2 Structure of a high-mass star-forming envelope (Chapters 3 and 4)

**Submillimeter spectral imaging** In order to study the effect of a high-mass protostar on its circumstellar material, I investigate the large-scale (~10^4–10^5 AU) physical and chemical structure of the molecular envelope of AFGL2591, with a bolometric luminosity of 2×10^4 L_{⊙} at a distance of 1 kpc. In chapter 3, a total of 35 spatially resolved spectral signatures are examined, extracted from JCMT Spectral Legacy Survey (SLS, 330–373 GHz) observations. Substructure is found in maps of, e.g., CO, N_{2}H^{+}, o-H_{2}CO, CS, C_{2}H, and CH_{3}OH, most notably a double-peak structure in warm methanol, indicative of a secondary heating source in the envelope.

I employ radiative transfer modeling to show that a spherical, static description of the envelope explains the observed intensity distribution of the optically thin tracers C^{34}S 7–6 and H^{13}CO^{+} 4–3, but runs into optical depth problems for optically thick lines such as HCN 4–3, CS 7–6, and HCO^{+} 4–3. The introduction of velocity structure in the form of infall mitigates the optical depth effects, but does not fully explain the observations. A static but flattened envelope viewed at a small inclination angle does slightly better, but is still not the ultimate answer. The conclusion is that the geometry of the envelope needs to be different from a homogeneous static sphere.

**Chemical inventory of the massive protostellar envelope** In addition, the SLS dataset of AFGL2591 is being explored further in the spectral dimension. On top of the 35 spatially resolved spectral signatures, more than 100 additional lines are identified in appendix 3.A. A similar inventory drawn up from the far-infrared CHESS spectrum will be added in the near future. The many lines of species such as CH_{3}OH and SO_{2} enable a detailed excitation analysis, whereas detections of rare isotopic species, including DCO^{+} and DCN, are probes of optical depth effects and the chemical history. A detailed comparison of observationally derived column densities and relative abundances with those predicted by chemical models for this source will constrain ideas about the chemical and physical evolution of high-mass protostars.
**Highly excited envelope gas** Next, chapter 4 studies high-$J$ lines of CO, HCN, HNC, CS and HCO$^+$ toward the same object, observed in a 490–1240 GHz spectral survey as part of the HIFI Key Program ‘Chemical Herschel Surveys of Star forming regions’ (CHESS). At these high frequencies, one probes energy levels up to $\sim 300$ K for these linear rotor molecules. The spectral resolution of $\sim 0.5 \text{ km s}^{-1}$ allows to disentangle two blended components in sufficiently bright lines: a broad component associated to outflow motion, and a narrower component associated to the quiescent envelope.

I derive a density and temperature for the outflow gas that are similar to those in the envelope (chapter 4.5.2), perhaps indicating that the material in the two components is mixed. In addition, the temperature of a known foreground cloud is constrained to $[9, \sim 15]$ K with an H$_2$ column density of a few $10^{21}$ cm$^{-2}$ (chapter 4.5.1).

In the envelope component, the peak position and line width manifest a shift with increasing upper level energy, which is attributed to a residual outflow contribution as sampled in the systematically decreasing telescope beam (chapter 4.3). Two radiative transfer models are set up for the envelope: a spherical one with constant molecular abundance, and one including an outflow cavity, direct UV illumination and shocked regions, which affect the local chemical balance. Comparing observations with these models (chapter 4.4), integrated line intensities of the highly excited lines observed here turn out to be surprisingly insensitive to the presence of outflow cavities. Modeling is ongoing for lines of HCO$^+$ and HCN, which are expected to be more sensitive to UV illumination and shocks. Distinctive observational probes of outflow cavities and shock physics are likely provided by even higher-$J$ lines of CO, up to $J=30$, as shown by, e.g., Van Kempen et al. (2010) for low-mass envelopes. Such observations are in fact planned for AFGL2591, using the PACS instrument on board *Herschel*.

**Inhomogeneity in molecular envelopes** It is worth to make an explicit connection between the results of chapters 3 and 4, where observed line emission is compared to radiative transfer models of the envelope. In the conclusions of chapter 3, I propose that the line optical depth in circumstellar envelope models could be alleviated by (i) combining infall and flattening, by (ii) adding an outflow cavity, and/or by (iii) introducing inhomogeneous structure. However, the first option is not preferred due to the lack of observable infall signatures (chapter 3.4.4). The second option can only be a partial solution, given the results from the cavity geometry employed in chapter 4.4.2, where I find indications that CO line emission up to $E_{\text{up}} \sim 300$ K is mostly sensitive to the cold, outer, spherical envelope. Hence, by elimination, the third option becomes ever more promising: inhomogeneous – ‘clumpy’ – structure in protostellar envelopes.

While observational evidence of substructure is compiled in this thesis and elsewhere (e.g., Wang et al. 1993; Lis & Schilke 2003), modern radiative transfer codes like $\beta3D$ and $LIME$ are capable of solving 3D-geometries (Poelman & Spaans 2005; Brinch & Hogerheijde 2010). With the combination of these numerical codes and modern computer power it is becoming feasible to take models of protostellar
7.3 Chemical stratification in the Orion Bar

envelopes one step further. Whereas most current studies of molecular environments are based on spherical or axial symmetry, a full 3D approach will now allow for inhomogeneous structure to be incorporated into protostellar envelope models. In fact, clumpy envelope structures have already been presented by Indebetouw et al. (2006) to create low-opacity paths for infrared continuum radiation. The extension from continuum to molecular line radiative transfer is natural.

Because the addition of inhomogeneous substructure introduces an extensive set of new free parameters to a model, I propose that an initial guess for the substructure could be derived from larger scale model simulations of molecular clouds. Hydrodynamical simulations, for example by Bate (2005) and Hocuk & Spaans (2010b), follow the collapse of the overall cloud and track the formation of clumpy structures leading to individual protostellar cores. It is feasible to adapt such a simulation to zoom in to $10^2$ AU scales with the aim of resolving substructure in an individual protostellar core.

It is important to anchor numerical modeling efforts in physical reality by directly comparing the model results to observations. For the spatial scales involved in the substructure I am proposing to model, interferometric (sub)millimeter facilities such as the PdBI, (e)SMA and ultimately ALMA will be essential to resolve subarcsecond structure. Even before the full 66-antenna ALMA array is operational, its superb sensitivity and angular resolution, combined with the broad frequency range (84–950 GHz) attainable from the dry Atacama desert, will transcend capabilities of all current millimeter/submillimeter facilities. At the same time, single-dish telescopes will remain important to efficiently map the distribution of molecular gas at larger scales.

7.3 Chemical stratification in the Orion Bar

(Chapter 5)

The copious amounts of UV-radiation emitted by young O- and B-stars have a profound effect on the atomic and molecular material in the surrounding ISM, for example in photodissociation regions (PDRs). One specifically suitable PDR to explore this effect is the Orion Bar, which is studied in chapter 5. I have used the first Orion Bar observations from the SLS program to study chemical stratification resulting from UV-radiation impinging on the Orion Bar. The observed layering is such that the C$_2$H radical lies close to the ionization front, and H$_2$CO, SO, C$^{18}$O, HCN, and $^{13}$CO are seen progressively deeper into the cloud. A simple gas-phase PDR model reproduces the observed layering, with the exceptions of the placement and abundances of SO and H$_2$CO. The conclusion is that depletion onto dust grains (of sulfur, for example) and production of H$_2$CO through grain surface chemistry should be incorporated in the models. Although the model used here is based on a smooth density structure, we also conclude that HCN and SO emission stems from high-density clumps, whereas CO traces the more tenuous interclump gas.
On the numerical modeling side, various groups are working on improvements of PDR codes. While not intending to provide an exhaustive listing of PDR modeling efforts, I mention two groups whose work is specifically relevant to the conclusions drawn in chapter 5 of this thesis. First, efforts are ongoing in Cologne to implement a clumpy layered geometry in the framework of the KOSMA-τ code (Röllig et al. 2006, 2011, in preparation). Second, a group in Groningen and Leiden (Meijerink, Cazaux & Spaans) is committed to the inclusion of grain surface chemistry of, e.g., H$_2$CO, into the PDR/XDR models of Meijerink & Spaans (2005).

As for the depletion of atomic sulfur and the impact on sulfur chemistry in PDRs, the conclusions in chapter 5 point to a sulfur depletion factor of more than 1000 in the Orion Bar. Previous work has already indicated that sulfur depletion factors span a large range of values between 4 and 1000 (e.g., Tieftrunk et al. 1994; Goicoechea et al. 2006). I have obtained follow-up spectral mapping of sulfur-bearing molecules toward a selection of other PDRs, to test the dependence of sulfur depletion on environmental factors such as the external UV irradiation level.

7.4 Methylidyne gas toward NGC6334 I
(Chapter 6)

For the study of quiescent gas toward the high-mass star-forming core NGC6334 I in chapter 6, I use Herschel/HIFI observations of the $J=\frac{3}{2}-\frac{1}{2}$ transition of methylidyne (CH), one of the earliest results from the CHESS program. The bolometric luminosity of NGC6334 I, at a distance of 1.7 kpc, is several $10^5 L_\odot$, about ten times more luminous than AFGL2591.

For the hot core itself, a remarkably low CH abundance of $7 \times 10^{-11}$ is derived, a factor of several hundred below that in diffuse clouds (Polehampton et al. 2005). In contrast with, e.g., H$_2$O (Emprechtinger et al. 2010), the CH gas in the hot core is inferred to trace quiescent material, not heated or dynamically influenced by outflow activity.

CH spectra generated by a code that calculates frequency-dependent optical depths and line brightnesses indicate that four absorbing foreground components are necessary to explain the observed spectrum. I derive column densities and line-of-sight velocities for these absorbing clouds. From counterparts in other molecular tracers, I conclude that two of the absorbing clouds are associated to the NGC6334 complex and that the other two are unrelated foreground clouds.

The results of chapter 6 demonstrate that the CH molecule is not just a tracer of diffuse interstellar gas, but that it also survives in dense, hot cores, acting as a probe of quiescent gas in an otherwise violent environment. While chapter 6 of this thesis is based on signatures of one rotational transition of a single molecule, the future exploitation of the extremely line-rich 490–1900 GHz CHESS spectrum of NGC6334 I is likely to yield many new results and generate new questions, especially concerning the fragmented hot core.