Physical and Chemical Structure of the Disk and Envelope of the Class 0/I Protostar L1527

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Abstract

Submillimeter spectral line and continuum emission from the protoplanetary disks and envelopes of protostars is a powerful probe of their structure, chemistry, and dynamics. Here we present a benchmark study of our modeling code, RadChemT, that for the first time uses a chemical model to reproduce ALMA C18O (2–1), and CARMA 12CO (1–0) and N2H+ (1–0) observations of L1527; this allows us to distinguish the disk, the infalling envelope, and outflow of this Class 0/I protostar. RadChemT combines dynamics, radiative transfer, gas chemistry, and gas–grain reactions to generate models that can be directly compared with observations for individual protostars. Rather than individually fit abundances to a large number of free parameters, we aim to best match the spectral line maps by (i) adopting a physical model based on density structure and luminosity derived primarily from previous work that fit spectral energy distribution and 2D imaging data, updating it to include a narrow jet detected in CARMA and ALMA data near (≤75 au) the protostar, and then (ii) computing the resulting astrochemical abundances for 292 chemical species. Our model reproduces the C18O and N2H+ line strengths within a factor of 3.0; this is encouraging considering the pronounced abundance variation (factor >100) between the outflow shell and CO snowline region near the midplane. Further, our modeling confirms suggestions regarding the anticorrelation between N2H+ and the CO snowline between 400 au and 2000 au from the central star. Our modeling tools represent a new and powerful capability with which to exploit the richness of spectral line imaging provided by modern submillimeter interferometers.

Unified Astronomy Thesaurus concepts: Protostars (1302); Radiative transfer (1335); Astrochemistry (75); Spectral line identification (2073); Star formation (1569); Molecular physics (2058)

1. Introduction

In star formation theory, a low-mass protostar in its earliest stage of the order of 10^5 yr, is considered a Class 0 newborn star embedded in a dense core typically containing a mass density of ~10^{-19} g cm^{-3} (Bergin & Tafalla 2007). During the rotational-collapse process at around 10^5 yr, the cloud conserves angular momentum, where the parts with low angular momentum form a protostar, while those with higher angular momentum settle into a disk in orbit around the protostar (Terebey et al. 1984); the gas and dust in the disk spiral inward through it and accrete onto the protostar.

Magnetic fields embedded in the initial cloud core can resist the collapse, and remove angular momentum by carrying the rotational energy of the core away into the surrounding molecular cloud. However, if the cloud is weakly ionized, its coupling to magnetic fields is slight, and magnetic fields can be ignored in the collapse. Several recent reviews suggest that magnetic fields may play a relatively small role during cloud collapse (Hull & Zhang 2019; Krumholz & Federrath 2019). When magnetic fields are negligible, the collapse conserves angular momentum along streamlines. The density structure in an initially quiescent, isothermal, collapsing core can then be described by the Ulrich envelope model (Ulrich 1976; Cassen & Moosman 1981, hereafter the UCM collapse model) or the inside-out Terebey–Shu–Cassen (hereafter TSC) collapse model (Terebey et al. 1984). These two models differ from each other in terms of gas pressure support and infall velocity, particularly outside the collapse radius (~4000 au, see Section 2.2.1). The whole picture of the protostellar system can be inferred from dust continuum and spectral line emission, where the age, luminosity, and mass of young protostar can be determined (Kenyon & Hartmann 1995; Evans et al. 2009; Dunham & Vorobyov 2012; Jørgensen et al. 2013; Frimann et al. 2016).

Predicting chemical abundances in envelopes and disks of protostars provides a way to trace the chemical inheritance of water and organics in planet formation; however, carrying out a realistic time-dependent chemical model using 2D physical properties is technically challenging. An early chemical study by Ceccarelli et al. (1996) assumed 1D (radial) physical structure for the envelope, and by determining temperature via radiative transfer, concluded that water would be abundant at temperatures above 100 K in protostellar envelopes. Other studies, also using 1D physical models with radiative transfer, further demonstrated the importance of temperature, from showing extreme CO depletion in cold outer envelopes, to the presence of simple organic molecules in corinos, namely regions of warm gas near the embedded protostar (Jørgensen et al. 2002, 2005; Ceccarelli et al. 2007; Yang et al. 2020). Time dependence in the chemistry has also been used to predict chemical signatures that result from episodic bursts of accretion in protostars (Jørgensen et al. 2015; Visser et al. 2015; Rab et al. 2017).

Subsequent studies have extended physical modeling from 1D to 2D (Visser et al. 2009, 2011; Drozdovskaya et al. 2014, 2016) and focus on the time history of a parcel of gas, in order to predict the abundance of species such as CO, water, and methanol within disks. Their conclusions on chemistry, while informative, are not compared with observations of protostars,
and moreover, make specific assumptions about luminosity evolution that are difficult to test.

However, for comparison with observation, the previous studies have limitations, and in particular, they do not model warm gas that is associated with outflows. Many molecules show strong emission from gas in outflows. For example, Kristensen et al. (2017) present data for a protostar sample observed with Herschel; the velocity data for water and high-$J$ CO lines show that these spectral lines are clearly associated with the outflow. In order to more reliably model molecules in the different spatial regions, a fully 2D description that includes outflow dynamics is necessary. In this contribution, our goal is to develop a fully 2D code that self-consistently predicts abundances for many molecular species in protostars, and moreover one that can be compared with high-spatial-resolution spectral line data from the Atacama Large Millimeter/submillimeter Array (ALMA). We try to be parsimonious in the model, to generate realistic results that include a simple outflow description, and that also minimize the inclusion of luminosity evolution, in order to better understand the importance of these effects. In this paper, we do not intend to find the best fitting parameters for the protostar L1527 but rather use what have been previously determined by Tobin et al. (2012) as initial parameters to explore the chemistry of the envelope in L1527 using RadChemT, which combines a physical model with a chemical one (see Sections 2.2.4 and 2.2.5 for more details).

We use the protostar L1527 to compare and validate our chemical model calculations produced by RadChemT (see Section 2.1 for more details of the utility of this package). L1527 is a typical dense core system classified as a class 0/I protostar with an edge-on disk orientation located 140 parsecs away in the Taurus molecular cloud (Beichman et al. 1986; Torres et al. 2007; Tobin et al. 2008; Kristensen et al. 2012). The edge-on orientation is favorable for studying the velocity structure of the envelope and outflow that is important to later constrain the mass of the protostar itself. Previous effort by Tobin et al. (2008, 2010, 2012) provided extensive fitting, through modeling and imaging, for the physical properties of the system, although the non-unique nature of spectral energy distribution (SED) fitting (Robitaille et al. 2007) means that there is still a wide range in free parameters to play with. More recently, Aso et al. (2017) constrained the radius and mass of L1527 using high-resolution data from ALMA.

Using RadChemT, we attempt to simultaneously match the observed C$^{18}$O (2–1), 12CO (1–0), and N$_2$H$^+$ (1–0) line strengths and position–velocity (PV) diagrams, together with continuum data at infrared through millimeter wavelengths. These molecules and transitions are of interest since they are widely detectable by submillimeter interferometers. 12CO is an abundant species having strong transitions, so it traces even the low-density gas in the outflow. C$^{18}$O probes regions of higher gas density (≥$10^3$ cm$^{-3}$) that are affected by photodissociation processes caused by ultraviolet (UV) photons close to the disk surface and is a very good tracer of the gas properties, structure, and kinematics (Visser et al. 2009). The rotational line emission of C$^{18}$O has a much lower optical depth than 12CO, and thus probes in more detail the inner parts of the envelope (Henning & Semenov 2013; Rab et al. 2017). Observations for some class I systems (Takakuwa et al. 2012, 2013, 2017; Harsono et al. 2013; Yen et al. 2013; Murillo et al. 2015) have shown that gaseous disks can be Keplerian, but understanding their formation relies greatly on what the spectral line emission is telling us. Moreover, non-Keplerian dynamics occurs in the cold outer disk boundary where the gas motion is free-falling onto the disk, shocks are expected, and there is the potential for a different structural gas flow (Sakai et al. 2014). N$_2$H$^+$ is one of the last species depleted in prestellar cores, and traces the coldest, densest material (∼$10^7$ cm$^{-3}$).

We present the first chemical calculations for L1527 using RadChemT. We provide a useful description of the physical parameters and the chemical model used to support the observations by Spitzer, Herschel, the Combined Array for Research in Millimeter-wave Astronomy (CARMA), and ALMA. As for the physical description of the model, we compare the UCM and the TSC collapse models and choose a density distribution to decide which one is more compelling to describe what is happening at the line center of the spectral data. We use the HOCHUNK3D code (Whitney et al. 2013) to determine the temperature using continuum Monte Carlo radiative transfer (MCRT). Then, we evolve a chemical network at each cell to find the molecular abundances, evaluating the regions dominated by the UV field, and finally construct synthetic spectral lines to compare against the interferometric data set. In Section 2.2 we describe in detail the setup of the physical model to simulate L1527 observations. In Section 2.3 we present the essentials to model the chemistry based on the temperature and density gathered from the physical model. In Section 2.4 we present the tools to produce images of L1527. In Section 3, we present the observational parameters of ALMA and CARMA. In Section 4 we present the results and discussions of the physical structure and chemical evolution using the tracers already mentioned earlier for L1527, and we outline the new CARMA data together with ALMA data for validation of the models. Finally, in Section 5 we present a summary of our findings.

2. Methods

2.1. RadChemT Overview

To make the modeling effort tractable, the software package we have assembled, RadChemT, breaks the calculation into three parts with several key simplifying assumptions. Step 1 carries out MCRT using HOCHUNK3D, as described in Section 2.2, to calculate dust temperature based on the current-time luminosity $L_{\text{int}}$ and 2D input physical model. Namely, for a given snapshot in time, both density $\rho(r, \theta, \phi)$ and velocity $v(r, \theta, \phi)$ are specified for the main components during the dynamical collapse of the class 0/I system: outflow, rotationally flattened envelope, and disk. The physical model is tuned to L1527, based on fitting modeling and imaging data from Tobin et al. (2008, 2010, 2012).

Step 2 performs a full time-dependent chemical abundance calculation in a point model, i.e., locally for each cell as described in Section 2.3, using the density and temperature from Step 1. As a simplification, this first version of RadChemT does not track material along a gas streamline as a function of time. Instead, the abundance calculations at each spatial grid point are time-dependent but assume fixed density and temperature. The assumption is that current local conditions ($\rho, T$) sufficiently describe earlier times. The assumption is most valid in the outer envelope, where density and temperature change the least for a moving gas parcel. There is an initial (brief) transient behavior in the chemistry, from starting with elements in atomic form, until molecular cloud abundances are achieved. After this, the
chemical age should be the same as the protostar age. The age of an individual protostar can be estimated using \( t_{\text{age}} = M_\odot/M_\text{env} \), but the age of an individual object is not well known during this early stage. We therefore compare chemical abundance and morphology at two time stamps, 10^4 and 10^5 yr, that roughly span the range of relevant ages for the Class 0/I phase. Predicted abundances that are relatively constant over that time span give confidence that conclusions based on those abundances will be robust.

Step 3 visualizes the protostar in a PV cube, making use of the Doppler effect in spectral line emission to sense the 3D velocity structure. This investigation uses RADMC-3D, as described in Section 2.4, to perform spectral line radiative transfer assuming LTE. The main inputs are the density, temperature, and velocity grids from Step 2, combined with an abundance grid from Step 1. From the inputs, RADMC-3D creates a synthetic model PV cube in FITS format having units of Jy pixel^{-1}. The primary and synthesized beams are then applied to the model spectral line cube, in order to compare the model with ALMA and CARMA submillimeter observations.

2.2. Physical Model: Modifications of HOCHUNK3D

The physical structure of our representative Class 0/I model is based on the HOCHUNK3D code (Whitney et al. 2013). This model uses an MCRT calculation to obtain the temperature of the dust and the gas density profile. The 2D geometry considers the system in spherical coordinates with axial symmetry and a logarithmically increasing grid in radius. The radial domain goes from the dust destruction radius, which is 10.04 \( R_\odot \), to the outer edge of the envelope, \( R_\text{env} = 12.500 \) au. The meridional domain covers the full 180°. The model includes a description of the density structure of the disk component and of the envelope with an outflow cavity. Figure 1 shows a schematic of the TSC geometry. Both the TSC and UCM models have similar parameters to tune; Table 1 tabulates adopted values for L1527 to be described more specifically in Sections 2.2.4 and 2.2.5.

We adopt a dust model that is appropriate for protostellar environments, based on a comparison of models with observations (Huard & Terebey 2017). Specifically we adopt the thinly ice-mantled, coagulated dust of Ossenkopf & Henning (1994) (see their Table 1, fifth column), often referred to as "OHS" grains in the literature (e.g., Evans et al. 2001; Shirley et al. 2005), augmented by the opacities of Pollack et al. (1994) at wavelengths shorter than 1.25 \( \mu \)m, as described in Dunham et al. (2010). In the next subsections we explain how the main components—envelope (Section 2.2.1), disk (Section 2.2.2), and outflow cavities (Section 2.2.3)—are structured in the model and the physical parameters (Sections 2.2.4 and 2.2.5) we chose to model L1527.

2.2.1. Envelope Prescription

Each region has its own density structure, and its distribution profile is semi-analytic. For the UCM collapse model we incorporate the density structure of the envelope as implemented in HOCHUNK3D. We use a separate calculation to determine the envelope density for the TSC collapse model (Terebey et al. 1984), which consists of an infalling, slowly rotating cloud that becomes rotationally flattened as it collapses. These two
The symbol : means the UCM values are the same as the TSC values. The envelope radius to collapse models are the same in the inner part of the envelope, but differ in the outer envelope due to the fact that UCM neglects gas pressure support. For both collapse models, we set the envelope radius to \( R_{\text{env}} \), and for the TSC model the infall velocity is zero outside \( \sim 4000 \) au, which is the current boundary of the infall region, and it moreover has an infall rate of \( 3.0 \times 10^{-6} \) \( M_\odot \) yr\(^{-1}\). But for the TMC model, the infall velocity in this outer region is not zero, but is given by the freefall velocity onto the 0.22 \( M_\odot \) protostar, with a mass infall rate of \( 5.0 \times 10^{-6} \) \( M_\odot \) yr\(^{-1}\); moreover, UCM neglects any acceleration from the massive envelope (see Huard & Terebey 2017 for additional discussion). Hence the UCM and TSC models presented here have different values for the density of the envelope, but the spatial grid, as well as the outflow and disk definitions, are the same for both models. We expect the difference between the UCM and TSC models to be greatest in the cold outer envelope, where the infall speeds are lowest, less than about five times the thermal sound speed (see Table 1). This cold gas contributes significantly to the emission near the core of the spectral line, within about 1 km s\(^{-1}\) of line center. The latter depends on the maximum recoverable spatial scale of L1527. The model comparison is meant to show whether the analytic UCM model is sufficient or whether it is necessary to include the additional complexity of the TSC model in order to match the spectral line profiles.

\[ \rho_{\text{disk}} \varepsilon_{\text{disk}} = \rho_{\text{env}} (c_{\text{env}}^2 + v_{\perp}^2), \]

where \( v_\perp \) represents the velocity component that is perpendicular to the disk midplane. The thermal sound speed is calculated assuming \( c_t = (kT/\mu m_p)^{1/2} \) and assuming that the dust and gas temperatures are equal, which is a reasonable assumption for protostellar densities. The disk shape that is found using this boundary condition is no longer that of a flared disk, but that of a disk with fairly constant opening angle out to its edge, as described in Section 4.

### 2.2.3. Outflow Cavities and Outflow Jet Prescription

We use the prescription of Whitney et al. (2003a) for the shape of the outflow cavity. The shapes of both outflow cavities are described by a polynomial function for L1527, which follows \( z(\varpi) = \varpi^b \) where \( \varpi = (\chi^2 + y^2)^{1/2} \) is the cylindrical radius and \( b = (\text{inner, outer}) = (1.7, 1.5) \) is the cavity shape exponent. \( \theta_1 \) and \( \theta_2 \) are the opening angles of the inner and outer cavity surfaces, respectively, defined at the maximum radius of the envelope. Only the apex of \( \theta_1 \) reaches the source center, and the apex of \( \theta_2 \) starts after 75 au. The density inside the outflow cavities is set to a constant value of \( 1.6 \times 10^{-20} \) g cm\(^{-3}\).

### 2.2.4. Parameters

Initial values for the parameters were based on the SEDs and image fitting done by Tobin and collaborators (Tobin et al. 2008, 2010, 2012, 2013). The modeling of L1527 is primarily sensitive to \( L_{\text{int}} \), which depends directly on the chosen values of \( R_s \) and \( T_s \) (see Table 1), the radius and temperature of the star, respectively. As described in Whitney et al. (2013), to determine the effective temperature of the star, we specify spot parameters such as: the number of spots at 45° in latitude is two, and the fractional area is 0.10. Defining \( R_s \) and \( T_s \), we keep the internal luminosity \( L_{\text{int}} = 2.74 L_\odot \) fixed, which is reasonable given the range of possible luminosity values for L1527. The mass of a Class 0/I protostar should be small. Therefore we looked at lower mass values in the literature, and selected a central star mass of \( M_s = 0.22 M_\odot \), a mass that best fits the position–velocity diagram for \(^{13}\)CO (Tobin et al. 2012). The disk outer radius is the centrifugal radius, which is set to 75 au (Aso et al. 2017). The disk inner radius is the dust destruction radius, a value that is set by the code depending on the stellar luminosity.

Two important considerations are crucial to matching both of the SED apertures, and for both TSC and UCM for our modeled L1527. Using identical parameters leads to somewhat different-looking SEDs; however we find that solely modifying \( M_{\text{env}} \) and \( M_{\text{disk}} \) brings the SEDs for UCM and TSC into reasonable correspondence, especially near 100 \( \mu \)m wavelength, near the far-infrared peak of the SED. In this case, the reasonable parameters found are \( M_{\text{disk}} = 0.006 M_\odot \) and however, as a first step toward including shocks we slightly modified the shape in which the disk–envelope boundary is defined in HOCHUNK3D by including a ram pressure boundary condition for motion perpendicular to the disk midplane. The assumption is akin to that of infalling material hitting a “brick wall” in the disk midplane. If the pressure is expressed in terms of the thermal sound speed as \( P = \rho c_s^2 \), and the ram pressure as \( P + \rho v^2 \), then the disk–envelope boundary is defined by matching the disk and envelope ram pressures:
$M_{\text{env}}$ of $5.0 \times 10^{-6} M_\odot \text{yr}^{-1}$ for the UCM model. For the TSC model, on the other hand, the mass of the disk chosen is $0.011 M_\odot$ with $M_{\text{env}}$ of $3.0 \times 10^{-6} M_\odot \text{yr}^{-1}$. The second consideration is the outflow; from newer data we find there is evidence in both the CARMA and ALMA $^{13}$CO data for a narrow jet, plus a wide-angle bipolar outflow, with a transition that happens at $\sim 75$ au from the protostar. The ALMA data (Figure 8) show the inner region, including the jet and outflow lobes in a representative velocity channel. The CARMA $^{12}$CO data in the channel maps of Figures 6 and 9 also display a narrow outflow structure near the protostar. We model this structure (Figure 3) using a dual outflow cavity with the narrow “jet” extending to 75 au, a radius that is similar to the 85 au suggested by a cavity modeling analysis from Tobin et al. (2010). We also specify a small but nonzero density in the outflow cavity ($1.6 \times 10^{-20} \text{ g cm}^{-3}$); adding a small amount of material (having standard dust-to-gas mass ratio of 0.01) to the outflow cavity produced a better fit to the SED than that shown in Tobin et al. (2010). Our choice of outflow parameters removes the need for the puffed-up disk required by previous modeling (Tobin et al. 2010). For the purposes of this paper we did not attempt a detailed modeling of the jet length or the cavity shape.

### 2.2.5. Luminosity

The internal luminosity is fixed at $L_{\text{int}} = 2.74 L_\odot$, to match the internal luminosity of 2.74 $L_\odot$ found by Tobin et al. (2008). The internal luminosity includes contributions from the star $L_{\text{star}}$, plus the accretion luminosity from material falling onto the star $L_{\text{acc,star}}$ and the accretion luminosity generated within the disk $L_{\text{acc,disk}}$, as described in Whitney et al. (2013). The mass of a Class 0/I protostar should be small and most of its luminosity should be due to accretion. This led to choosing a stellar radius of $1.70 R_\odot$ with an effective temperature of 3300 K, which gives a stellar luminosity of 0.31 $L_\odot$ (see Table 1). One additional term, $L_{\text{IRSF}}$, contributes to the total luminosity of the system, $L_{\text{tot}} = L_{\text{int}} + L_{\text{IRSF}} = 3.23 L_\odot$; the term $L_{\text{IRSF}}$ is due to external illumination by the interstellar radiation field (ISRF) and is based on the Galactic value computed near our solar system; see the description in Huard & Terebey (2017).

The largest luminosity term is due to the stellar hot-spot accretion luminosity, which is defined as

$$L_{\text{acc,star}} = GM_{\text{sh}} M_{\text{disk}} \left( \frac{1}{R_*} - \frac{1}{R_{\text{trunc}}} \right) \quad (2)$$

where $R_{\text{trunc}}$ is the truncation radius where the disk is truncated by the stellar magnetospheric field, and its value is approximately the same as in Tobin et al. (2008). The disk accretion rate $M_{\text{disk}}$ is an important parameter that leads to the stellar accretion luminosity, which encompasses about 66% of the total luminosity of the system. The code determines that the value $M_{\text{disk}} = 6.6 \times 10^{-7} M_\odot \text{yr}^{-1}$ leads to an accretion luminosity onto the star of 2.14 $L_\odot$.

We also include the disk accretion luminosity in terms of the energy dissipated at the inner boundary of the disk (see Shakura & Sunyaev 1973; Lynden-Bell & Pringle 1974; Kenyon & Hartmann 1987; Whitney et al. 2003b, for more details). Table 1 summarizes the values of the different luminosity terms.

### 2.3. Chemical Model

We model the local chemical evolution to determine the abundances of the molecules that have been observed. The chemical models are time-dependent, and we focus on the results at two epochs, 10^6 and 10^7 yr, that span the range of possible ages for L1527.

Our chemical network is taken from the UMIST database, RATE12 (McElroy et al. 2013). The reactions of the carbon and oxygen isotopes have been added such that each reaction involving an atom of the major isotopes will have an equivalent reaction involving the minor isotopes (see Willacy & Woods 2009, for more details). Fractionation of the oxygen and carbon isotopes can occur via the reactions listed in Table 2. For reactions involving $^{17}$O the values of $\Delta E$ are taken to be the same as for the equivalent reaction of $^{18}$O, and the pre-exponential part of the rate calculation is scaled by the reduced mass (Young 2007).

![Table 2](attachment:image.png)

| Reaction | Reaction | $\Delta E$ |
|----------|----------|------------|
| $^{13}$C$^+$ + CO $\rightarrow$ C$^+$ + $^{13}$CO | $\Delta E = 35$ K |
| $^{13}$C$^+$ + $^{18}$O $\rightarrow$ $^{13}$CO + $^{18}$O | $\Delta E = 36$ K |
| $^{13}$CO + H$^+$ $\rightarrow$ C$^+$ + $^{13}$CO$^+$ | $\Delta E = 9$ K |

Note. $\Delta E$ values are taken from Langer et al. (1984). $\Delta E$ values for reactions involving $^{17}$O are assumed to be the same as for the equivalent reaction of $^{18}$O, with the pre-exponential factor in the rate calculation scaled by the reduced mass (Young 2007).

The network also includes gas–grain reactions, i.e., freezeout on the grain (Hasegawa & Herbst 1993), thermal desorption (Hasegawa et al. 1992), as well as photodesorption, and desorption by heating of grains by cosmic rays (Öberg et al. 2009a, 2009b). The freezeout and desorption reactions are also described in Woods & Willacy (2009). Freezeout is assumed to occur with a sticking coefficient of 1.0 (Bisschop et al. 2006) for all species. For desorption processes, the binding energies required are taken from UMIST12. Cosmic-ray heating rates are given by

$$k_{\text{crh}} = 3.16 \times 10^{-19} \times \exp(-E_b/70 \text{ K}) \quad (3)$$

(Hasegawa & Herbst 1993), where $E_b$ is the binding energy of the accreted molecule. Photodesorption rates are given by

$$k_{\text{phond}} = FY (\pi a^2 n_x) \Theta_X \quad (4)$$

(Willacy & Langer 2000) where $F$ is the UV field (the total of the stellar, interstellar, and cosmic-ray-induced fields in units of $G_0$), $Y$ is the yield per photon, which is taken to be $10^{-3}$ for all
species (Westley et al. 1995), except for oxygen atoms ($Y = 10^{-5}$) and $\text{H}_2\text{O}$ ($Y = 10^{-3}$) and $Y = 2 \times 10^{-5}$ for description as OH (Hollenbach et al. 2009). The dust is assumed to be well mixed with the gas, $n_g$ is the number density of dust grains ($n_g = 10^{-12} n_H$), and the average $\langle \pi a^2 n_g \rangle = 2.1 \times 10^{-21} n_H$ (standard interstellar value). $\Theta_X$ is the surface coverage of species $X (= n(X)/\Sigma n(Y)$, where $n(X)$ is the abundance of $X$ in the ices and $\Sigma n(Y)$ is the total abundance of ices). The stellar UV field is assumed to have a typical T Tauri value of 500 $G_0$ at 100 au (unextincted) from the star, where $G_0$ is the standard ISRF (Bergin et al. 2003). The dense envelope generates significant extinction. To account for this, the local UV field is decreased to take into account the extinction calculated along the line of sight to the star.

Grain surface reactions are included using the approach of Garrod & Pauly 2011. Only atoms, $\text{H}_2$, and simple hydrides (OH, CH, NH, and their isotopologues) are assumed to be mobile on the grain surface.

Initially we assume that all elements are in their atomic form, except for carbon which is ionic and hydrogen which is 95% molecular. The initial abundances used are given in Table 3. We assume a cosmic-ray ionization rate of $\zeta_{\text{CR}} = 1.3 \times 10^{-17} \text{ s}^{-1}$.

For the photodissociation of CO (and its isotopologues) and $\text{H}_2$ we use the self-shielding coefficients provided by Visser et al. (2009) assuming a Doppler width of 0.3 km s$^{-1}$ and isotopic ratios of $^{12}\text{C} / ^{13}\text{C} = 89$, $^{16}\text{O} / ^{18}\text{O} = 498$, and $^{16}\text{O} / ^{17}\text{O} = 1988$, which are taken to be the same as values in the local interstellar medium (Wouterloot et al. 2008). Abundances here are prescribed as $X$, the fractional abundances relative to total hydrogen, $n_X / (n_H + 2n_H)$. For $^{12}\text{C}$, $^{13}\text{C}$, $^{16}\text{O}$, $^{17}\text{O}$, and $^{18}\text{O}$.

| Species | $X$ |
|---------|-----|
| H       | $1.00 \times 10^{-2}$ |
| $\text{H}_2$ | 0.495 |
| He      | 0.140 |
| C       | 7.22 $\times 10^{-5}$ |
| $^{13}\text{C}$ | 8.11 $\times 10^{-7}$ |
| N       | 2.14 $\times 10^{-5}$ |
| O       | 1.75 $\times 10^{-4}$ |
| $^{17}\text{O}$ | 8.80 $\times 10^{-8}$ |
| $^{18}\text{O}$ | 3.51 $\times 10^{-7}$ |
| Si$^+$  | 2.00 $\times 10^{-8}$ |

$^*$ $X$ is the fractional abundance relative to hydrogen, $n_X / (n_H + 2n_H)$.

2.4. Synthetic Line Images

Step 3 of RadChemT calculates the protostellar environment in a PV cube. Because HOCHUNK3D did not include spectral line emission we selected RADMC-3D, version 0.41 (Dullemond et al. 2012), to generate synthetic spectral line emission assuming LTE. LTE improves computational speed and holds in locations where the gas density is above the critical density. The generation of synthetic line images takes into consideration the density, temperature, and velocity grids from Step 1, and the abundance grid from Step 2 at $t = 10^5$ yr and $t = 10^7$ yr time stamps, all of which are translated into the RADMC-3D file format.

Finally, for each model density distribution and epoch, we carry out line-of-sight radiative transfer calculations using RADMC-3D to construct synthetic line and continuum observations, and compare these against the multi-telescope data set for L1527.

Additional inputs for L1527 in RADMC-3D were source inclination $i = 85^\circ$, distance $d = 140$ pc, and system velocity $v_{\text{sys}} = 6.0$ km s$^{-1}$. For consistency the OHS dust opacity law is the same as that used for the Step 1 continuum radiative transfer. Standard and reasonable assumptions for the protostellar environment are $T_{\text{dust}} = T_{\text{gas}}$ and 100 for the gas-to-dust ratio. The microturbulent velocity was fixed at 0.1 km s$^{-1}$, a value that is required for LTE and results in smoothing the line profile. A larger microturbulent velocity could affect the hyperfine structures of the molecular spectrum by causing line blending. However, data from CARMA CO observations indicate that somewhat larger values for the microturbulence should be used for the outflow shell region. Based on the $^{12}$CO data presented in Section 4.5.1 and in Appendix C, we chose a very simple outflow velocity prescription having a constant outward radial motion of 3 km s$^{-1}$ in the outflow cavity and also in the outflow shell. However, a careful treatment of the outflow shell lies outside the scope of this paper. From the inputs RADMC-3D creates a synthetic model PV cube in FITS format that has units of Jy pixel$^{-1}$.

Comparison with observations also requires applying telescope-specific parameters. The velocity channel width and spatial pixel size were specified as inputs to RADMC-3D. The synthetic images are sampled in real space in order to be able to see more clearly the variations in the chemical abundances, and therefore the dynamical range of the system, which in our models are greater than the interferometric data. To compare with millimeter interferometer data, the synthetic model images are multiplied by a Gaussian primary beam (peak value normalized to unity), and then convolved with a circular Gaussian synthesized beam (area normalized to unity). See Section 3 for ALMA and CARMA observational parameters.

3. Observations

3.1. CARMA Data

L1527 was observed in 2009 August and November using CARMA, which is located at an altitude of 2200 m on the Eastern California Inyo mountains. Observations were obtained...
in D- and C-array configurations, which provide a uniform \( \nu \)-coverage between 9 and 371 m. The CARMA correlator was set to observe the \(^{12}\text{CO} \ (1-0)\) emission line (\( \nu = 115.271 \text{ GHz} \)) in the upper side band, and the \(^{13}\text{CO} \ (1-0)\) (\( \nu = 110.201 \text{ GHz} \)) line in the lower side band. These two lines were observed at a velocity resolution of 0.34 km s\(^{-1}\) in two 8 MHz spectral windows. The dust continuum emission was observed in two 1 GHz windows separated by 3.6 GHz and centered at the mean frequency of 112.73625 GHz (\( \lambda = 2.66 \text{ mm} \)). Here we do not use \(^{13}\text{CO} \ (1-0)\) since it has higher optical depth than \(^{12}\text{CO} \), making it more difficult to see the emission from the disk. The bandpass shape was calibrated by observing 3C 84, and the flux calibration was set by observing Uranus. The quasar 3C 11 was observed every 12 minutes to correct for atmospheric and instrumental effects. The data reduction and the image reconstruction were obtained using the MIRIAD software package. For \(^{2}\text{H}\) data and model comparison, we convolve the model using a geometric mean FWHM of 9", namely, \( b = \sqrt{b_{\text{max}} \times b_{\text{min}}} = \sqrt{10.97'' \times 8.73''} = 9''. \) The observational parameters are listed in Table 4.

### 3.2. ALMA Data

The observational data presented for \(^{18}\text{O} \ (2-1)\), which have a spatial resolution of 0.96" \( \times \) 0.73" (that is the geometric beam) and a maximum recoverable scale of \( \sim 15'' \), are based on data from the ALMA archive that were taken during cycle 0 on 2012 August 26 (Project code: 2011.0.00210.S). ALMA data with higher spatial resolution exist, but they resolve out much of the \( \sim 10'' \) emission that is relevant to this study. We convolve the model using the same geometric mean formulation as in CARMA, giving \( b \approx 0.8 '' \) for the ALMA spatial resolution. The model is also multiplied by the ALMA primary beam, which was taken to be a smooth 28'' FWHM Gaussian image. Table 5 summarizes observational parameters. More information about the observations and calibration is given in Table 1 in Ohashi et al. (2014).

### 4. Results and Discussions

#### 4.1. L1527 SED Fits

We present a comparison of the flux density of the simulated L1527 for both UCM and TSC models. The simulated L1527 SEDs are shown in Figure 2 plotted at 85° edge-on (pink), the appropriate inclination of L1527 (Oya et al. 2015). Panels (a) and (b) show the model SEDs computed for a 1000 au (7''14) aperture and a larger 10,000 au (71''4) aperture, respectively. We also include a plot to illustrate the strong effect of source inclination on the SED model curves. We re-generate SEDs for L1527 by including the flux density values from Tobin et al. (2008) plus we added flux density values from Herschel (see Tables 6 and 7), which come mostly from the thermal radiation of the envelope. The Herschel data were downloaded from the IRSA/IPAC archive. Since the Herschel CDF spectrum (Green et al. 2016) and the flux density points in the HPPSC catalog (Marton et al. 2017) have apertures of 6–14", i.e., they lie in between the model 7''14 and 71''4 apertures, we chose to show the Herschel data on both SED aperture plots. Although we do not intend to redo the best parameter fit for L1527, here we revisit the outskirts of the envelope, where the emission is also important for the chemistry.

Overall, both the UCM and TSC models provide reasonable SED fits, with the TSC model providing a better fit for the 10,000 au aperture that is consistent with the large spatial extent of the system. Another regime that supports our later statement is the region where the disk emits, which is between 2.16 and 8.0 \( \mu \)m. We find that the TSC is a closer fit to the flux points, although not perfectly due to the different dust opacity, population, and density that exist here, which are not necessarily in accordance with the dust opacity model we use for the envelope. The PACS data are also of particular interest because they occur near the peak of the SED. The Herschel PACS HPPSC data have an aperture of 6" at 70 \( \mu \)m and 100 \( \mu \)m, and 12" at 160 \( \mu \)m. The PACS data at 70 \( \mu \)m and 100 \( \mu \)m have a spatial resolution that is comparable with that of the 7''14 aperture model (Figure 2(a)), and moreover, the flux density values do not deviate much from the modeled ones. However, for PACS > 100 \( \mu \)m the resolution is slightly offset since the discrepancy in aperture size is greater. The Herschel spectrum does not match the Herschel photometry points either, so the Herschel data are not consistent with each other at around 100 \( \mu \)m and longer wavelengths. Some possible explanations are that (a) the source is extended, which might mean the data are affected by jet emission; (b) the source is varying in luminosity (source variability).

The properties of the central region were chosen carefully (see Section 2.2.4) to best describe the physical structure of L1527 as constrained by imaging data and the SED photometry. We estimated these stellar properties properly describing L1527 based on Tobin et al. (2008, 2010, 2013). We also adjusted the description of the outflow cavity to transition from jet to wide-
angle outflow based on ALMA CO data (Figure 8) at 75 au (see Section 2.2.4). For the fixed protostellar parameters listed in Table 1 and described in Sections 2.2.4 and 2.2.5, we varied the mass infall rate and disk mass, finding the mass infall rate, $M_{\text{env}}$, to be $5 \times 10^{-6} M_\odot \text{yr}^{-1}$ and $3 \times 10^{-6} M_\odot \text{yr}^{-1}$ for the UCM and TSC models, respectively. Based on the magnitude of $M_{\text{env}}$ chosen, the age of the simulated L1527 is estimated to be $\sim 7 \times 10^4 \text{yr}$. We adopt that L1527 is in the protostar collapse phase with an age of $t \approx 10^5 \text{yr}$.

To further assess the self-consistency of the model, we note that in every evolutionary stage of the star formation process, the mass budget of the infalling envelope and accreting disk have to be consistent with the feedback of the outflows and winds. In the absence of any outflow, $M_{\text{env}} = M_{\text{disk}}$, all of which falls onto the central star. As discussed in Section 2.2.5 and shown by Equation (2), the disk accretion $M_{\text{disk}}$ leads to generous $L_{\text{acc,\star}}$ accretion luminosity, which is fit by the modeling procedure. Therefore a mismatch in the two accretion rates is related to outflow feedback. The infall efficiency is given by the ratio of the accretion rates; for L1527 our model value of $M_{\text{disk}}/M_{\text{env}} = 6.6 \times 10^{-7} M_\odot \text{yr}^{-1}/3 \times 10^{-6} M_\odot \text{yr}^{-1} = 0.22$. We point out that this value is similar to the value of 0.25 estimated for the protostar TMC-1 (Terebey et al. 2006). These values differ from unity, and provide interesting constraints on theoretical discussions of star formation efficiency. See Matzner & McKee (2000), and in the context of high-mass star formation, Zhang et al. (2014) for an extensive treatment of outflow feedback and its relation to star formation efficiency.

Next, for comparison with van ’t Hoff et al. (2018), we produced a second UCM run by increasing the stellar mass to $0.45 M_\odot$ and the disk radius to 125 au. The untuned model produced SED fits that were worse but still reasonable. No significant difference could be discerned in the density, temperature, or resultant chemistry. However, the velocities increased by a factor of 2 due to higher gravity from the larger mass. The effect was clearly seen in model spectral line profiles and PV diagrams (see further in Section 4.5.2), thus making it a promising way to investigate the dynamical mass of L1527 in future studies.

### 4.2. Temperature and Density Maps

Figure 3 presents the dust temperature (top panels) and gas density (bottom panels), computed using the RadChemT package, as meridional cuts through the envelope + disk + bipolar outflow cavity. Views on three different scales are shown from left to right.
The central star is located at the origin, the outflow cavities extend horizontally, and the edge-on disk (vertical) is oriented 90° with respect to the outflow cavities. The dust temperature is calculated from the radiative equilibrium solution using HOCHUNK3D and its distribution varies as the power-law function of the radius, $T \sim r^{-0.5}$ in optically thick regions, and as the power $r^{-0.33}$ in optically thin regions (Kenyon et al. 1993). Near the protostar, the temperature increases due to exposure to stellar radiation in this region, making it feasible for the atomic gas to be present at vibrational energy levels. The radius of the collapsing region (i.e., expansion wave) is 3800 au, and grows larger in time at the sound speed. Outside the collapse radius, the density distribution becomes flat, transitioning to smaller radius to the freefall zone where the density behaves as $\rho \sim r^{-3/2}$ well outside the disk (Shu 1977; Terebey et al. 1984). Contour lines in white show $T = 25$ K (top panels), our definition of the evaporation temperature of CO (e.g., Qi et al. 2015, 2019; Wiebe et al. 2019), and number density $n = 10^5$ cm$^{-3}$ (bottom panels). The shape of the dual outflow cavity is seen most clearly in the middle density plane in blue; near 75 au the narrow outflow/jet opens into a wide-angle outflow. The circle in the lower right shows the (small) 1000 au radius aperture ($7''$) that is used for aperture photometry. Note that this aperture covers a small portion of L1527, making it necessary to compare PACS data points with 71'' (10,000 au), which covers a much larger region.

The outer disk radius equals the centrifugal radius of the envelope, 75 au, and the disk–envelope boundary is wedge-shaped due to the ram pressure boundary condition (see Section 2.2). The region of highest density is found at the disk midplane with the number density of the order of $\sim 10^{14}$ cm$^{-3}$. In this region of high density inside 50 au, the temperature in the disk midplane is slightly higher than 30 K. Beyond 75 au, the midplane is shielded from the stellar radiation, leading

molecules to gradually freeze out onto dust grains until $T = 25$ K at $\sim 225$ au, where the CO snowline lies and freeze-out is expected to happen more rapidly. Beyond the $T = 25$ K contour line, the temperature decreases until it reaches the typical temperature of the envelope, $T = 10$ K. Since we do not include shocks, there is no increase in the temperature profile due to them. The luminosity that shocks can produce is a small fraction of the stellar luminosity; however, it is been suggested that can be enough to liberate molecules from grains (Sakai et al. 2014). Comparing the UCM and TSC models, the temperature and the density distributions of both show very little difference in terms of structure.

### 4.3. $^{13}$CO Abundance Distribution

The timescale for freeze-out onto grains depends on both the temperature and density (Hartmann et al. 2004), which vary throughout the cloud. The chemistry at the outer boundary of the cloud is determined by the low temperature, low density, and exposure to the ISRF. Within the cloud envelope, at first the rapid increase of density inward dominates, so that molecules freeze out onto grains in regions of low temperature and high density. Nearer the protostar the temperature rises above the desorption temperature, at which point the behavior changes, and molecules come off the grains and are released
into the gas phase. The chemistry is also affected by the UV radiation field from the protostar. Dust extinction shields regions near the midplane from the protostellar UV field.

The dense gas distribution is often traced using isotopologues of CO, such as C\textsuperscript{18}O, which are less likely to be optically thick than CO itself. For both time steps, \( t = 10^4 \) yr and \( t = 10^5 \) yr, high C\textsuperscript{18}O abundances (\( \sim 10^{-7} \) relative to hydrogen) primarily come from the disk and envelope at radii smaller than 400 au, where the temperature is 25 K (see Figure 3) and the chemistry can be dominated by thermal desorption reactions and perhaps photodesorption reactions due to the capture of stellar radiation. Due to the lower abundance and optical depth of C\textsuperscript{18}O, the effect of photodissociation is visible as a drop of \( 10^\times \) in C\textsuperscript{18}O abundance already in the outer envelope (\( \sim 8000 \) au) at \( t = 10^5 \) yr. But in terms of spatial extent, the C\textsuperscript{18}O is similar to \( ^{12}\text{CO} \), as seen in Figure 4(a), but different for absolute abundance. We found no significant difference between UCM and TSC models for chemical abundances, and therefore limit the discussion to the TSC model abundances.

Our chemistry matches expectations in the envelope outside the edge of the disk, where we expect lower concentrations of C\textsuperscript{18}O (\( \leq 10^{-8} \)) due to the high-density area that is shielded from stellar radiation, and thus it is cooler in this region. An abundance gap in the midplane beyond 300 au is present for both \( t = 10^4 \) yr and \( t = 10^5 \) yr, and is consistent with the depletion expected in the region beyond the CO snowline (\( T \leq 25 \) K) in the disk and envelope midplane. At \( t = 10^5 \) yr there is a steep drop in the C\textsuperscript{18}O abundance between 400 au and 4000 au due to the short freeze-out timescale compared with the outermost part of the cloud, where the freeze-out timescale becomes longer (i.e., Caselli et al. 1999).

In the outermost region in the envelope (\( r > 4000 \) au), the temperature drops to \( T \approx 10 \) K; the light enhancement of C\textsuperscript{18}O abundance (\( \sim 10^{-8} \)) in this region is influenced by photodesorption reactions such as cosmic rays coming from outside the cloud.

The chemistry results presented here for \( ^{12}\text{CO} \), C\textsuperscript{18}O, and also for \( \text{N}_2\text{H}^+ \) (in Section 4.4) represent a small subset of molecular abundances that are available for comparison with observations. Our RadChemT model includes a chemical network that provides abundance predictions for 292 chemical species; this number includes carbon and oxygen isotopologues and 90 grain surface abundances, a promising area for further studies.

4.4. \( \text{N}_2\text{H}^+ \) as CO Snowline Tracer

Snowlines, such as those for water and CO, are important because they can influence the efficiency of planet formation within the cold shielded regions of disks. Because CO line emission is optically thick, which makes it difficult to observe the dense interior regions, recent studies by Aikawa et al. (2015) and van ’t Hoff et al. (2017) suggest that it is necessary to derive the location of the CO snowline from \( \text{N}_2\text{H}^+ \) observations. Observations have established that the \( \text{N}_2\text{H}^+ \) abundance is anticorrelated with CO abundance in systems
Figure 4. Evolution of (a) $^{12}$CO and (b) $N_2H^+$ gas-phase abundances, both for the TSC model. In (a), the black contour line shows the maximum $^{12}$CO abundance divided by 10. In (b), the black contour line shows the maximum $N_2H^+$ abundance, also divided by 10. The purple dashed line in the first panel shows the disk. The maximum CO abundance is $7.22 \times 10^{-5}$. The color bar is on a logarithmic scale.
ranging from starless cores (i.e., Tafalla et al. 2004), to class 0 protostars (i.e., Jørgensen 2004), to protoplanetary disks (i.e., Qi et al. 2013, 2015, 2019; Wiebe et al. 2019).

Our chemistry results show a general predicted trend, that gas-phase $^{12}$CO and N$_2$H$^+$ are anticorrelated in the envelope. In the upper middle and right panels of Figure 4(a), at $t = 10^3$ yr the $^{12}$CO is depleted from the gas phase, and at $t = 10^4$ yr (lower middle and right panels) the $^{12}$CO depletion region increases outward. The increase in N$_2$H$^+$ concentration, beyond 400 au, is consistent with the $^{12}$CO depletion to $t = 10^3$ yr (Figure 4(b), lower middle and right). Inside 320 au, $^{12}$CO is enhanced since $T > 25$ K in this region (see the first two top panels in Figure 3) due to thermal and photodesorption reactions whereas N$_2$H$^+$ is absent. Therefore, the $^{12}$CO snowline is present and the best anticorrelation takes place at $T \sim 25$ K in the midplane.

The predicted anticorrelation covers a larger region at $t = 10^3$ yr, which is the nominal age of L1527, and shows that the N$_2$H$^+$ concentration grows and extends from 400 au to $\sim 2000$ au (close to the midplane). The N$_2$H$^+$ is present in the outer envelope at larger abundances at $t = 10^3$ yr than at $t = 10^4$ yr. Thus, our models show a general predicted trend, that gas-phase $^{12}$CO and N$_2$H$^+$ are anticorrelated in the envelope. Although the CO depletion timescale differs somewhat from the N$_2$H$^+$ growth timescale, the increase in N$_2$H$^+$ abundance should closely follow the slow depletion of $^{12}$CO since gas-phase timescales are much shorter than freeze-out timescales. The chemistry models are thus consistent with N$_2$H$^+$ being a good tracer for the $^{12}$CO snowline. Note that the abundances in the outflow cavity are excluded from consideration (see Section 2.3). The jagged boundary between outflow cavity and envelope is due to grid sampling effects mentioned in Section 2.3.

4.5. Spectral Line Comparison: Models versus Observations

In order to compare our models with observations, we generate synthetic model spectral line images of N$_2$H$^+$ for CARMA and compare their anticorrelation with $^{12}$CO CARMA data (Section 4.5.1). In order to convey the validation of RadChemT, we generate a synthetic spectral line for C$^{18}$O, from which we extract synthetic PV diagrams to compare with ALMA observations (Section 4.5.2). Each model spectral line data cube is based on the density, temperature, velocity grids, and chemical abundances analyzed in previous sections.

4.5.1. N$_2$H$^+$ and $^{12}$CO CARMA

Figure 5 presents the RadChemT model in the form of an integrated intensity map of N$_2$H$^+$ at $t = 10^3$ yr. The best N$_2$H$^+$ and $^{12}$CO anticorrelation takes place at $t = 10^3$ yr, where the greater extent of the N$_2$H$^+$ abundance (see Figure 4(a)) is more consistent with the CARMA data than at $t = 10^4$ yr. In Figure 5 we predict the spatial extent of the N$_2$H$^+$ intensity. By not convolving the modeled emission of Figure 5 with the beam, we are able to see in more detail the spatial structure of the N$_2$H$^+$ emission in the envelope, otherwise the X-shape emission would partially disappear and look more like a vertical bar, very similar to how it looks in Figure 6(a). As previously discussed in Section 4.4, the predicted N$_2$H$^+$ emission traces cold dense gas in the envelope between 400 au and $\sim 3000$ au, extending north–south along the midplane. The predicted emission is seen to peak north and south of the protostar position, with less emission at $\leq 400$ au, or about 3" in radius, where Figure 4 predicts that N$_2$H$^+$ should be absent. Although less visually prominent, there is also extended N$_2$H$^+$ that corresponds to the outer envelope, which is faintly seen in Figure 5 at the level of $\sim 0.002$ Jy pixel$^{-1}$, extending across the simulated image.

The N$_2$H$^+$ spectrum is constructed by integrating over the entire 10,000 au image, and this includes and confirms the hyperfine components seen in Figure 6(b). The red solid line (model) and green plus symbols (data) show good correspondence at $t = 10^3$ yr. Note that the extended (faint) emission contributes significantly to the predicted spectrum. For the two emission peaks from the inner envelope (two red peaks in Figure 5), there is a discrepancy between the spatial extent of our prediction (Figures 4 and 5) and the observation (Figure 6), which we conjecture might be improved by increasing the collapse age of the system in terms of changing the dynamics so that $R_{col}$ leads to a larger collapsing region. This is a good motivation to follow a time-dependent evolutionary parcel and thus confirm the spatial extent. Overall, the strength of the observed N$_2$H$^+$ emission is consistent with the model prediction as seen in the spectrum.

Figure 6 also presents the integrated intensity maps of $^{12}$CO (1-0) from CARMA that cover the same 71″4 (10,000 au) field of view and which show outflowing CO gas that extends east–west, perpendicular to the N$_2$H$^+$ emission. The dust continuum emission (red contours) is centered on the protostar position. In $^{12}$CO a narrow “jet” extends east–west from the protostar, merging into a wide-angle outflow on both sides of the protostar position.
protostar. The narrow “jet” is also confirmed by ALMA (Figure 8), therefore supporting the inclusion of an inner outflow jet in our model. Figure 9 in Appendix C contains the $^{13}$CO velocity channel maps, which further show that the emission arises in an ($\pm 3 \text{ km s}^{-1}$) outflow shell. None of the emission extends north–south, since the high optical depth of $^{12}$CO blocks any meaningful view of the low-velocity envelope.

We conclude that the N$_2$H$^+$ emission shows evidence for the predicted anticorrelation with $^{12}$CO. The N$_2$H$^+$ appears to be missing within 400 au of the protostar, just where full-strength $^{13}$CO emission is predicted. One difference is that our predicted emission is less extended than the data (Figure 5), which extends out to $\sim 30''$ ($\sim 4200$ au). However, the data agree in showing N$_2$H$^+$ enhancement at $\pm 18'' \sim 2500$ au from the protostar, where the model predicts there is severe depletion for $^{12}$CO (see Figure 4). A factor that might help to further improve the comparison is to increase $R_{\text{col}}$ and follow the evolutionary process of the chemical parcel spatially.

4.5.2. C$^{18}$O ALMA

We focus on C$^{18}$O (2–1) observations from ALMA in order to investigate the kinematics of the dense gas distribution in the disk and inner envelope in a spectral line tracer that is (nearly) optically thin. The orientation of the rotating and infalling material extends north–south (as seen in Figure 1) and C$^{18}$O probes dense gas near the protostar. The edge-on inclination of L1527 means that a north–south cut along the midplane will minimize the contamination of the dense gas emission by the outflow. However, the central 0''8 beam, meaning $\pm 0''4$ centered on the protostar, can still contain some outflow emission. The $^{12}$CO emission (Figure 8) for a region of the same size is optically thick and traces gas of lower density extending east–west in the outflow shell.

To compare with the ALMA data we make a synthetic model spectral line cube that matches the ALMA data file. That is, we generate velocity channel maps for C$^{18}$O (2–1) with a velocity spacing of 0.167 km s$^{-1}$ and pixel size of 0''17. We convolve the model with the 0''8 effective beam, and apply the 28'' primary beam, as described in Section 2.4. Note that RadChemT includes a basic description of the outflow velocity prescription of 3 km s$^{-1}$ in the model, since RadChemT self-consistently computes the abundances of both $^{12}$CO and C$^{18}$O as well as the radiative transfer of the two species (LTE is assumed).

The edge-on inclination of L1527 means that a PV diagram is well suited for viewing the kinematics of rotation and infall in the central envelope and disk. Figure 7 presents PV diagrams for C$^{18}$O (2–1), where panel (a) shows the ALMA data that are also presented in Ohashi et al. (2014). These data are sampled in real space to clearly see the cloud features in more detail. Panel (b) shows the simulated L1527 as modeled using the TSC model, and panel (c) shows it as modeled using the UCM model. Each horizontal row in Figure 7 corresponds to a spectrum that is spatially offset from the protostar in the north–south direction. The horizontal solid white line marks the position of the protostar, which is located at 0'' offset. The effective width of the position slice is the 0''8 beam ($=112$ au at 140 pc) and the units are Jy beam$^{-1}$. The vertical solid white line shows the adopted 6.0 km s$^{-1}$ Doppler radial velocity of L1527.

The data (panel (a)) show that C$^{18}$O is self-absorbed at the protostar position, where the solid white lines meet at the center of the PV diagram. This indicates that the C$^{18}$O is optically thick at line center, consistent with the finding of van ’t Hoff et al. (2018). However, our model does not currently reproduce the self-absorption feature, seen to occur within $\pm 0.5$ km s$^{-1}$ from line center (6.0 km s$^{-1}$). In a later paragraph we further discuss the self-absorption. The data (panel (a)) also show an artifact that is common to interferometers. The cloud emission from L1527 is
spatially extended and therefore resolved out by the interferometer at the 6.0 km s\(^{-1}\) cloud velocity, resulting in no or little emission from the cloud near the vertical line. However, the RadChemT images retain the low-velocity cloud emission at 6.0 km s\(^{-1}\), and do not mimic this artifact of the data. At large spatial offsets (>4″) the spectral line has a narrow width that approximates the thermal sound speed of the cloud. The range of velocities \(v\) in each spectrum (i.e., horizontal row) increases toward the protostar (i.e., smaller \(R\) and smaller position offset), as is expected for gravitational motion where \(v \sim \sqrt{GM/R}\). The emission occurs mainly in the lower left and upper right quadrants, which is the expected signature of rotational motion in a disk. Emission that occurs in the “forbidden” quadrants (upper left and lower right) is not from the rotating disk, but instead is a signature of the rotating and infalling envelope (i.e., Ho & Keto 2007).

Comparison of the PV diagrams in Figure 7 shows an overall correspondence of the data with the RadChemT models that is

**Figure 7.** Position–velocity diagrams that show the velocity of \(^{13}\)CO vs. position offset along the north–south direction. Each horizontal row corresponds to a spectrum at the indicated spatial offset. Panel (a) shows the ALMA \(^{13}\)CO observational data. The PV diagram obtained from the RadChemT chemical model is shown in panel (b) for the TSC collapse model and panel (c) for the UCM collapse model. The white solid line in each panel shows the system radial velocity (vertical) and central protostar position (horizontal). Dashed white lines represent ±125 au, the maximum disk size considered. Keplerian rotation curves are included for reference. The solid black line represents the fiducial model with \(M_*=0.22\ M_\odot\) and \(R_{\text{disk}}=75\ \text{au}\). The dashed black line is \(M_*=0.45\ M_\odot\) and \(R_{\text{disk}}=125\ \text{au}\). Panels (b) and (c) show different color scale bars due to the higher density of UCM in the inner envelope. Panel (d) shows the \(^{13}\)CO (2–1) spectrum, integrated over a 3.4″×3.4″ box centered on the protostar. Green plus symbols are ALMA data; red triangles show the RadChemT TSC collapse model, multiplied by a 3.0× scaling factor.
encouraging. Visually, the TSC model (panel (b)) is a better fit than the UCM model (panel (c)). One difference between data and model is that the peak brightness values are symmetric in the models but not symmetric in the data. The data (panel (a)) show stronger blueshifted peak emission (lower left quadrant) than redshifted (upper right quadrant), which is a signature of optically thick emission. To improve the model fit, this suggests that the model envelope density (or abundance) should be increased above the fiducial value.

Recent analyses of L1527 in the literature using different data sets find $M_* = (0.19, 0.45, 0.45 M_\odot)$ and $R_{\text{disk}} = (125, 75, 125)$ au, respectively (Tobin et al. 2012; Aso et al. 2017; van ’t Hoff et al. 2018). In our fiducial model we adopted the values of Tobin et al. (2012) of $M_* = 0.22 M_\odot$ and $R_{\text{disk}} = 75$ au as a starting point to test the capabilities of RadChemT in reproducing the chemical abundances of L1527. Our fiducial numbers fall at the lower end of recent determinations. The analysis by van ’t Hoff et al. (2018) is the most similar to our modeling, although it assumes but does not compute the astrochemical abundances, and moreover restricts attention to the inner $\sim 1''$ (140 au).

In all three PV diagrams, the dashed white line represents the maximum size of the disk. Everything outside the dashed white lines, at $>1''$ position offset, is emission coming purely from the envelope. The emission coming from inside these lines is therefore due to a combination of envelope and disk emission. Keplerian rotation curves are presented as a guide for the eye, and represent the maximum velocity expected from a rotating Keplerian disk. The solid black line represents the fiducial model with $M_* = 0.22 M_\odot$ and $R_{\text{disk}} = 75$ au. The dashed black line is $M_* = 0.45 M_\odot$ and $R_{\text{disk}} = 125$ au, a model that is considered in van ’t Hoff et al. (2018). Comparison of the model PV diagram with the data in Figure 7 suggests that the higher protostar mass would be preferred over the fiducial value. However, detailed model fitting of the disk dynamics lies outside the scope of the current work.

The strength of the observed C$^{18}$O (2–1) emission is about a factor of 3.0 higher than the model prediction for the TSC model. Figure 7(d) shows the C$^{18}$O spectrum that is constructed by integrating over a $3''$ box (475 au $\times 475$ au). The red triangles (model) and green plus symbols (data) show reasonable correspondence in terms of profile shape. The overall emission of the UCM model is about 50% brighter; this difference is understandable as being due to the higher density of UCM in the inner envelope for our choice of physical parameters; an approximate estimate of the density ratio expected between UCM and TSC is 5/3, and is simply obtained from the ratio of $M_{\text{env}}$ values that are given in Table 1.

The fact of not reproducing the self-absorption at the protostar position in our modeled C$^{18}$O spectrum does not preclude the ability of the models to explain what is happening at the center of the spectral line. The observed self-absorption is consistent with a high-density region, grains with millimeter size or greater, in the disk that suggests a promising avenue for future studies to increase the density between the envelope and disk. Considering a different type of dust opacity that is more suitable for the inner parts is also encouraging. On the model processing side, performing the spectral tracing using non-LTE may also lead to improvement. In summary, the RadChemT model was not tweaked to match the C$^{18}$O emission, so the initial match between model and data to within the factor of 3.0 is encouraging.

From Figure 7 we see that our prediction of C$^{18}$O using the TSC model is better at representing the actual envelope structure of L1527 than C$^{18}$O ALMA data. Due to the fact that UCM neglects pressure effects in the outer layers of the envelope, we see that at spatial offsets $>1''$ (150 au), the UCM envelope shows too much gas at higher velocity, resulting in a rectangular rather than bowtie shape around the green perimeter, which shows the fainter emission. In general, we conclude that the predicted C$^{18}$O (2–1) emission from the RadChemT model reproduces the main features of the PV diagram (Figure 7) for both the envelope and disk emission. Moreover, these initial results suggest that RadChemT can be used as a tool to investigate the dynamical mass of the protostar, the disk radius, and the unknown dynamics of the outer disk. Future improvements to RadChemT to specifically model L1527 better could include: (1) increasing the density and opacity profile in the disk and performing non-LTE spectral line radiative transfer (i.e., Evans 1999), (2) changing the physical conditions as a function of time to follow collapse motions, and (3) including shock physics and adding sulfur chemistry to study the suggested enhancement of SO at the disk–envelope interface.

5. Summary and Conclusions

RadChemT is a method for modeling embedded protostars to compare with both continuum and molecular line observations. The method combines a two-dimensional axisymmetric cloud collapse solution, which varies with both distance from the star and angle from the rotation axis, with MCRT and the solution of an astrochemical reaction network. The resulting gas-phase abundances are transformed via LTE radiative transfer into simulated position–velocity cubes to compare with observational data on spectral lines. This pilot study with RadChemT uses a model of the central star and surrounding gas density distribution obtained by Tobin et al. (2008, 2010, 2012) for the protostar L1527. In the current implementation, a protostar of a given age has steady density and temperature distributions, while the chemical abundance calculation is time-dependent. There are pronounced spatial variations in the abundances. Abundances are enhanced in the outflow shell and decreased in the cold regions near the midplane, varying by more than a factor of 10$^3$ in the case of CO. In order to validate RadChemT, we generate PV diagrams for the inner 1000 au (14'') and compare with ALMA C$^{18}$O observations. We also present CARMA data for $^{12}$CO and N$_2$H$^+$ on a larger 10,000 au scale, and compare with our predicted abundances for L1527. We report our highlights as follows.

1. The TSC and UCM collapse models give comparable fits to the SEDs, for aperture sizes of both 10,000 au and 1000 au. Similarly, there is little qualitative difference in the predicted molecular abundances. However, the TSC model better corresponds to the observed PV diagrams. In the case of UCM, which neglects pressure forces, the envelope shows too much gas at higher velocity, particularly at spatial offsets greater than 150 au.

2. The ALMA C$^{18}$O (2–1) spectrum is about 3.0 times brighter than our C$^{18}$O prediction. This is reasonable agreement given that the astrochemical computation has not been “tuned” to improve the fit. However, increasing the density in the envelope and the opacity profile in the disk could be fruitful, since the C$^{18}$O abundance is sensitive to them. The dynamics of the C$^{18}$O gas imply that the protostar mass and disk radius are somewhat larger than the fiducial values of 0.22 $M_\odot$ and 75 au, respectively.
3. The CARMA $^{12}\text{CO}$ (1–0) data confirm that there is strong emission with the morphology of an outflow shell. The ALMA $^{12}\text{CO}$ (2–1) data definitively establish that a narrow jet-like structure connects the two outflow lobes inside 75 au. For the physical model we therefore include a swept-up outflow shell with a constant outward velocity of 3 km s$^{-1}$ (Figure 9) as a proof of concept. The chemistry implies that the $^{12}\text{CO}$ abundances are low in the inner envelope for $400 \text{au} < R_{\text{env}} < 2000 \text{au}$ at $t = 10^5$ yr, indicative of freeze-out onto grains.

4. In the CARMA $\text{N}_2\text{H}^+$ (1–0) data, emission is elongated north–south, with the peak emission offset $\sim 10''$ from the central star. In our chemical model, $\text{N}_2\text{H}^+$ is also offset, by about $\sim 10''$ north of the central star. This is indirect but strong evidence of significant $^{12}\text{CO}$ freeze-out in the same region. As found in many previous studies, the chemistry implies that $\text{N}_2\text{H}^+$ is anticorrelated with CO abundance. In the case of L1527, RadChemT predicts that $\text{N}_2\text{H}^+$ is enhanced in the envelope over 500 au $< R_{\text{env}} < 2000 \text{au}$ at $t = 10^5$ yr.

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Appendix A

$^{12}\text{CO}$ (2–1) ALMA Channel Map

The inner outflow/jet considered in the physical model is evidenced by the ALMA $^{12}\text{CO}$ data at 9.9 km s$^{-1}$.

Appendix B

CARMA $^{12}\text{CO}$ Channel Maps

Same as Appendix A. Evidence in the CARMA $^{12}\text{CO}$ data at different channels shows the same inner outflow/jet transitioning into a wide opening outflow cavity.

Appendix C

Initial Abundances

The elemental abundances used in the chemical model are shown in Table 4. We assume that all elements are in their atomic form except for carbon, which is in ionic form, and hydrogen, which is 95% in molecular form.

Appendix D

ALMA Observational Parameters

This is a summary of the ALMA C$^{18}$O observational parameters used for the chemical analysis. For more details see Ohashi et al. (2014).

Appendix E

Photometry

The flux points in the SEDs of L1527 were obtained from Tobin (2008), Table 1. The photometric and aperture information is shown in Table 6 and Table 7, with the references listed in the last column accordingly.

Figure 8. Snapshot of a $^{12}\text{CO}$ (2–1) ALMA channel map at 9.9 km s$^{-1}$ that shows the inner region of the outflow. The $^{12}\text{CO}$ emission is shaded in white and shows two outflow shells lying in the east–west direction that are connected by a narrow jet. This orientation matches Figure 1(b). The data have a spatial resolution of 0.98″ and the star position is at the center of the 10″ (1400 au) image.
Figure 9. $^{12}$CO CARMA channel maps. Contours are spaced by $3\sigma = 0.187$ Jy beam$^{-1}$. The lower left inset shows the FWHM beam size of $10'' \times 8''$. Each panel is $110'' \times 110''$. The radial velocity of L1527 is $6$ km s$^{-1}$; several blank velocity channels near $5$ km s$^{-1}$ suggest absorption due to a foreground cloud. In $^{12}$CO a narrow “jet” extends east–west from the protostar, merging into a wide-angle outflow on both sides it. The $^{12}$CO velocity channel maps show that the emission arises in an $(\pm 3$ km s$^{-1}$) outflow shell.

References

Aikawa, Y., Furuya, K., Nomura, H., & Qi, C. 2015, ApJ, 807, 120
Aso, Y., Ohashi, N., Aikawa, Y., et al. 2017, ApJ, 849, 56
Beichman, C. A., Myers, P. C., & Emerson, J. P. 1986, ApJ, 307, 337
Beichman, C. A., Neugebauer, G., Habing, H. J., Clegg, P. E., & Chester, T. J. 1988, Icar, 73
Bergin, E., Calvet, N., D’Alessio, P., & Herczeg, G. J. 2003, ApJ, 591, L159
Bergin, E. A., & Tafalla, M. 2007, ARA&A, 45, 339
Bisschop, S. E., Fraser, H. J., Öberg, K. I., van Dishoeck, E. F., & Schlemmer, S. 2006, A&A, 449, 1297
Caselli, P., Walmsley, C. M., Tafalla, M., Dore, L., & Myers, P. C. 1999, ApJ, 523, L165
Cassen, P., & Moosman, A. 1981, Icar, 48, 353
Ceccarelli, C., Caselli, P., Herbst, E., Tielens, A. G. G. M., & Caux, E. 2007, in Protostars and Planets V, ed. B. Reipurth, D. Jewitt, & K. Keil (Tucson, AZ: Univ. Arizona Press), 47
Ceccarelli, C., Hollenbach, D. J., & Tielens, A. G. G. M. 1996, ApJ, 471, 400
Chandler, C. J., & Richer, J. S. 2000, ApJ, 530, 851
Drozdovskaya, M. N., Walsh, C., van Dishoeck, E. F., et al. 2016, MNRAS, 462, 977
Drozdovskaya, M. N., Walsh, C., Visser, R., Harsono, D., & van Dishoeck, E. F. 2014, MNRAS, 445, 913
Dullemond, C. P., Juhasz, A., Pohl, A., et al. 2012, RADMC-3D: A multipurpose radiative transfer tool, Astrophysics Source Code Library, ascl:1202.015
Dunham, M. M., Evans, N. J. L., Terebey, S., Dullemond, C. P., & Young, C. H. 2010, ApJ, 710, 470
Dunham, M. M., & Vorobyov, E. I. 2012, ApJ, 747, 52
Evans, N. J. I. 1999, ARA&A, 37, 311
Evans, N. J. I., Rawlings, J. M. C., Shirley, Y. L., & Mundt, L. G. 2001, ApJ, 557, 193
Evans, N. J. I., Dunham, M. M., Jørgensen, J. K., et al. 2009, ApJS, 181, 321
Frimann, S., Jørgensen, J. K., Padoan, P., & Haugbølle, T. 2016, A&A, 587, A60
Garrod, R. T., & Pauly, T. 2011, ApJ, 735, 15
