Modeling CO Line Profiles in Shocks of W28 and IC 443

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Abstract

Molecular emission arising from the interactions of supernova remnant (SNR) shock waves and molecular clouds provides a tool for studying the dispersion and compression that might kick-start star formation as well as understanding cosmic-ray production. Purely rotational CO emission created by magnetohydrodynamic shock in the SNR–molecular cloud interaction is an effective shock tracer, particularly for slow-moving, continuous shocks into cold inner clumps of the molecular cloud. In this work, we present a new theoretical radiative transfer framework for predicting the line profile of CO with the Paris–Durham 1D shock model. We generated line profile predictions for CO emission produced by slow, magnetized C shocks into gas of density \(10^5\) cm\(^{-3}\) with shock speeds of 35 and 50 km s\(^{-1}\). The numerical framework to reproduce the CO line profile utilizes the large velocity gradient (LVG) approximation and the omission of optically thick plane-parallel slabs. With this framework, we generated predictions for various CO spectroscopic observations up to \(J = 16\) in SNRs W28 and IC 443, obtained with SOFIA, IRAM-30 m, APEX, and KPNO. We found that CO line profile prediction offers constraints on the shock velocity and pre-shock density independent of the absolute line brightness and requires fewer CO lines than diagnostics using a rotational excitation diagram.

Unified Astronomy Thesaurus concepts: Supernova remnants (1667); Interstellar medium (847); Magnetohydrodynamics (1964); Radiative transfer (1335)

1. Introduction

Believed to be the site of cosmic-ray enhancements, supernova remnant (SNR) shocks provide a possible explanation for the excess cosmic-ray photons and increased ionization rates in observations of SNR–molecular cloud interactions (Drury & Strong 2017). Understanding cosmic-ray origin and enhancements in SNRs provides an understanding of the SNR energy budget and production mechanisms of mega-electron-volt-tera-electronvolt cosmic rays. Analyses have been carried out extensively for SNR such as W28, with ROSAT X-ray observations (Rho et al. 1996), or the \(\gamma\)-ray observations with CANGAROO (Rowell et al. 2000). A more recent study by Phan et al. (2020) has also shown the cosmic-ray spectrum in the northeastern W28 is best explained by cosmic-ray protons from hundreds of mega-electronvolts to tens of tera-electronvolts. The interaction of SNR and molecular clouds thus are top laboratories for constraining the cosmic-ray spectrum across the Galactic plane.

Shocks into molecular clouds are laboratories for tracing the exchange of energies in the interstellar medium (ISM). Supernova shock waves carve cavities in the ISM and excite the molecular and atomic gas to higher temperatures. The gases act as coolants for the shocks, providing tracers of physical and chemical properties within molecular clouds. Observing the interactions in SNRs also provides clues about the supernova progenitor, particularly within the innermost layers of the supernova ejecta and the inferred mass and nucleosynthesis profiles (Temim et al. 2019).

The Paris–Durham MHD-shock model (Gusdorf et al. 2008a; Lesaffre et al. 2013; Flower & Forêts 2015; Tram et al. 2018; Godard et al. 2019) is an integrated toolkit for studying shocks. As the Paris–Durham shock unambiguously predicts the excitation diagram (or Boltzmann diagram, the relation between the column density of excited levels and excitation energy), previous studies of shocks have relied on observing multiple transitions of the same molecule in a region (see, e.g., Gusdorf et al. 2012; Lee et al. 2019) and comparing them with either single (e.g., van der Tak et al. 2007) or multiple gas temperatures and densities (e.g., Le Bourlot et al. 2002).

Tracing shocks with molecular spectroscopy is of great importance given their roles in diffusing molecular clouds and also compressing parts of the clouds and potentially triggering star formation. The slow, continuous shocks (C type; Draine et al. 1983; Draine & McKee 1993) have shown to be particularly important for explaining the existence of OH masers due to their non-dissociative nature: the resulting thick, warm, broad shock front allowed for efficient cooling compared to the thin layers of dissociative jump shocks (J type) (Warflake & Yusef-Zadeh 2002). Such interactions are observationally constrained by molecules. The Paris–Durham shock code can explicitly predict the velocity-resolved profile (or line profile) for an optically thin line such as \(H_2\) (e.g., Reach et al. 2019) or an optically thick line such as SiO (see, e.g., Gusdorf et al. 2008a, 2008b).

Carbon monoxide \((^{12}\text{C}^{16}\text{O})\) is among the most abundant molecules in the ISM, second only to diatomic hydrogen \((H_2)\). In contrast with \(H_2\), CO can be excited in low-temperature (even under 10 K) and low-density gas (even under \(10^3\) cm\(^{-3}\)), including the range of temperatures and densities expected for dense cores in molecular clouds (10–100 K and \(10^5\) cm\(^{-3}\), respectively). The pure rotational transitions \((J = 1)\) of the CO molecule cover far-infrared to submillimeter wavelengths.
Critical Density of CO for Pure Rotational Transitions

| $J_{\text{up}} - J_{\text{low}}$ | $v_{\text{up}} - v_{\text{low}}$ (GHz) | $n_{\text{crit}}$ (10 K) (cm$^{-3}$) | $n_{\text{crit}}$ (50 K) (cm$^{-3}$) |
|-----------------|-----------------|-----------------|-----------------|
| 2 → 1           | 16.60           | 230.54          | 9.7 × 10$^{3}$  | 1.2 × 10$^{4}$  |
| 3 → 2           | 33.19           | 345.79          | 3.2 × 10$^{2}$  | 3.8 × 10$^{2}$  |
| 5 → 4           | 82.97           | 576.27          | 1.8 × 10$^{5}$  | 1.7 × 10$^{5}$  |
| 9 → 8           | 248.88          | 1036.91         | 1.0 × 10$^{6}$  | 8.8 × 10$^{5}$  |
| 11 → 10         | 364.97          | 1267.01         | 1.6 × 10$^{6}$  | 1.5 × 10$^{6}$  |
| 13 → 12         | 503.13          | 1496.92         | 2.2 × 10$^{6}$  | 2.2 × 10$^{6}$  |
| 16 → 15         | 751.72          | 1841.35         | 3.5 × 10$^{6}$  | 3.5 × 10$^{6}$  |

Note. Calculated from the Leiden Atomic and Molecular Database (LAMDA) as a ratio of radiative coefficient and collisional coefficient ($n_{\text{crit}} = A_{ij}/C_{ij}$, where $H_2$ is the main collision partner $n_{H_2} = 1 \times 10^4$ cm$^{-3}$). Zero indexing is used. Pure rotational lines ($\Delta J = \pm 1$) of CO trace both cool and dense gas as well as hot gas in shocks, indicated by the excitation temperature and critical density for collisional excitation. High-J CO lines specifically indicate regions of denser, colder CO concentration.

These complements H$_2$ as an observational tracer, with CO emission lines capable of tracing the cold, dense gas (see Table 1) that could provide insight into star-forming cores (Burton 1987; van Dishoeck et al. 1993).

In this work, we expand the theoretical line profile modeling to CO, devise a custom numerical radiative transfer integration scheme from shock models, and apply it to new CO observations in IC 443 and W28—two pristine sites for studying the interaction between shocks and molecular clouds (illustrated in Figures 1 and 2).

This paper is organized as follows: in Section 2, we review observational constraints in SNR W28 and IC 443 and present new spectroscopic observations with SOFIA in the W28 BML4 region (broad molecular emission region). In Section 3, we discuss the theory of magnetohydrodynamic (MHD) shock and the setup of a priori Paris–Durham shock models. In Section 4, we discuss the associated theoretical radiative transfer framework and the relevant numerical scheme. In Section 5, we apply the framework to generate the line profile prediction of various CO observations to constrain shock properties, such as pre-shock density and shock velocity.

### 2. Nature of Shocks in W28 and IC 443

#### 2.1. Shocks in W28

W28 is a mixed-morphology SNR, among the brightest in radio and γ-ray emission (Giuliani et al. 2010; Green 2019). The region where shocks interact with the dense interstellar clouds is complex, with evidence of shocks into gas with a range of densities, including molecular shocks shown in Figure 1 (Reach et al. 2005). Its mixed morphology is seen by the contrast between the nonthermal radio shell structures versus thermal X-ray emission from the interior and requires an age greater than 10$^3$ yr (Rho & Petre 1998) and more likely of order 4 × 10$^4$ yr (Giuliani et al. 2010). Multiwavelength studies from submillimeter (Dubner et al. 2000; Vaupré et al. 2014) to X-ray (Zhou et al. 2014) and γ-ray have progressively revealed different aspects of the supernova–molecular cloud interaction and acceleration of cosmic rays (Cui et al. 2018). Pannuti et al. (2017) studied optical lines and X-ray sources in the interior of W28 and found evidence for oxygen-rich ejecta, suggesting that its progenitor star was massive. Furthermore, they pointed out that X-ray sources near the center of the SNR are unlikely to be remnants of the progenitor.

Strong evidence of the interaction of SNR blast wave with dense gas in the northern ridge of W28 has been presented by millimeter detection of a 1720 MHz OH maser in W28 (Claussen et al. 1997). Using millimeter and near-infrared detection of rotational/rovibrational lines of CO, CS, and HCO$^+$, H$_2$, and atomic lines, Reach et al. (2005) gave an estimate of $n($H$_2$) $\sim 10^3$–$10^5$ cm$^{-3}$ for the density of observed regions in W28, based on the observation of the broad molecular line (BML) regions, and they inferred that a large fraction of mass of the molecular clouds lies in a relatively compact volume. The observed SiO line width (∼21 km s$^{-1}$) and brightness also provided a lower limit of shock velocity at $V_s \gtrsim 20$ km s$^{-1}$. Furthermore, Reach & Rho (1996) calculated the line ratios of CS(2–1)/CO(2–1) ∼ 0.04 and CS(3–2)/CS (2–1) ∼ 1.0, which further constrained the excitation condition to $T \sim 100$ K and $n($H$_2)$ $\lesssim 10^4$ cm$^{-3}$.

More recent observation of various rotational CO lines with SOFIA-GREAT toward the location of maser OH(F) has revealed multiple overlapping shocked components, suggesting propagation into a complex cloud structure spanning multiple ranges of densities. Gusdorf et al. (2012) made use of multiple rotational lines to build a shock-predictive excitation model. The excitation diagram methods in Gusdorf et al. (2012) involved observing six CO lines of both $^{13}$CO and $^{12}$CO and predicting shock density using the excitation of each rotational level computed by a non-LTE radiative transfer with a single density-temperature input. Best-fit models indicate a stationary C-shock configuration, with $n = 10^4$ cm$^{-3}$ at an age of 10$^4$ yr. To explain the line width, the sum of two shock velocities and an ambient gas layer is used: $V_{\text{shock}} = 20$ and 25 km s$^{-1}$ with magnetic field components $b = 0.4$ and 1, or 40 and 100 μG, respectively. Projections effects are suggested to be the explanation for the difference in the two values. An upper estimate of post-shock density at $3 \times 10^3$ cm$^{-3}$ increases the magnetic field strength to 550 μG. The lower velocities limits are a consequence of the 1D nature of the model and the lack of direct constraints in the line profile.

In this work, we combine archival observations with new SOFIA observations of W28 BML4, at the J2000 coordinates 18:01:40.3–23:25:03, the brightest region of CO(2–1) emission (Reach et al. 2005). Observations were made using the German REceiver At Terahertz frequencies (GREAT; Risacher et al. 2018) on 2018 May 23, from an altitude of 40,000 feet, as part of program 06_0001. Figure 3 shows the new spectra of CO(1 = 16–15), O I (3P$_{\text{m}=2}$–1) at 63 μm, and C II (3P$_{\text{m}=3}$–2/1–2/1) at 158 μm. The properties of spectral lines from the new SOFIA observations are summarized in Table 2, and those from archival observations are summarized in Table 3. All of these lines showcase similarly broad line widths, as seen with low-J CO observations in the same region. Additionally, the unmatched central velocity peaks of high-J CO and low-J CO (10 and 5 km s$^{-1}$, respectively) in this region likely suggest different origins of shock, as previously observed in clump F of W28 by Gusdorf et al. (2012). It could be seen by comparing the centers of the CO(16–15) observation with the CO(2–1) observation from Reach et al. (2005) (see Figure 3). The line ratio of ⟨C II⟩/⟨O I⟩ $\sim 5$ provides a constraint on the range of a priori shock fits.
Figure 1. False color image (RGB with band VLA(P) 90 cm, MSX 8 μm, VLA(L) 20 cm) of the SNR W28 and its northern shocked ring (Brogan et al. 2004). The northeastern, dashed polygon indicates the region of the overlaid CO(2–1) map (Reach et al. 2005) with the 12 m ARO Telescope on Kitt Peak (KP12). The positions of five BML regions are shown.

Figure 2. Wide-field Infrared Survey Explorer IR false color image of SNR IC 443 (bands W4 22 μm, W2 4.6 μm, and W3 12 μm) and its entire shock rings. Overlaid is the contour map of the 2.1 μm H₂ emission from Burton (1987) for the ω-shaped southern ridge, with shocked clumps positions indicated.
2.2. Shocks in IC 443

IC 443 is another example of a supernova explosion adjacent to molecular clouds, which produces shock interactions across a range of densities. X-ray studies have revealed the compact stellar remnant of the progenitor of IC 443 to be a neutron star (Olbert et al. 2001; Swartz et al. 2015). An extremely well-studied object, IC 443 is a textbook example of shock–molecular cloud interaction.

Its morphology is mixed, with pristine shell-like structures where shocks interact with molecular clouds in the northeastern and southwestern regions, all indicated by emission from X-ray, submillimeter, and infrared as shown in Figure 2. An early study by van Dishoeck et al. (1993) revealed that shocks mainly occur at dense regions forming a flat ring shape in the southern portion of the SNR. The observations in the submillimeter are best explained by shocks into clumps of gas, each accelerated differently based on the densities. There is evidence that shock into high-density gases is a potential accelerator of cosmic rays up to teraelectronvolt energies, through the correlation of γ-ray observation and shock into molecular gas.

The pre-shock material likely takes a range of densities from lower-density outer shells to higher-density cores. Observations and theoretical modeling support the presence of gas with pre-shock density $\sim 10^{3}–10^{4}$ cm$^{-3}$ in the southern ridge of IC 443. Observations of H$_2$ and CO emission (Burton 1987; van Dishoeck et al. 1993; Cesarsky et al. 1999; Rho et al. 2001) revealed clumps of various densities within IC 443, whose pre-shock properties are mainly probed with excitation models. Mid-IR 6.9 µm observation and modeling of the H$_2$ S(5) prediction by Reach et al. (2019) further strengthen a similar range of pre-shock density using direct H$_2$ line profile fitting. In this work, we made use of CO observations from van Dishoeck et al. (1993) and Rho et al. (2001) in concordance with shock properties predicted with various molecular line emissions.

An age estimate by Troja et al. (2008) based on X-ray analysis is $t \sim 4000$ yr, while Chevalier (1999) optical observations put it as being much older at $t \sim 30,000$ yr. However, more recent efforts of theoretical modeling of 1D MHD shock for infrared observation (Reach et al. 2019) and 3D shock for X-ray observation (Ustamujic et al. 2021) both supported age estimates in the range of $t \sim 3000–8000$ yr. In this study, we employed a similar range of age estimates of 3000–10,000 yr.

3. MHD-shock Modeling

Draine & McKee (1993) review interstellar shocks in the interstellar medium, in which supernova explosions are among the major sources. In the rest frame of the shock, its structure can be divided into three regions: the pre-shock region, the radiative zone, and the post-shock region. The pre-shock material is heated and ionized by upstream (precursor) radiation and cosmic rays. As it reaches the shock transition, deceleration in flow velocity occurs (in the shock rest frame). In the radiative zone, kinetic energy is transferred into thermal energy, and entropy increases strongly. The post-shock gas
cools down as it moves further from the shock, where gas and dust could be irradiated by photons that propagated far downstream.

In scenarios such as the interaction of shock fronts with molecular clouds, strong magnetic fields are usually present. The Paris–Durham shock model\(^1\) (Gusdorf et al. 2008a; Flower & Forrest 2015; Godard et al. 2019) enables modeling for such magnetic-dominated shocks by assuming that the B field is transverse to the direction of propagation.

For two-fluid shocks, the magnetic fields are responsible for separating the flow into a neutral flow, and ionic flows that experience magnetic drag, coupling to the magnetic fields. Despite taking up a small fraction in mass, ionic flows strongly affect shock dynamics. For two-fluid shocks, three types of solutions are possible: C (continuous shock), J (jump shock), and a mixed CJ (or C\(^*\)), depending on whether the shock transitions smoothly from super- to subsonic speed as it decelerates (Draine et al. 1983; Draine & McKee 1993).

We generated four a priori C-shock models to investigate the resulting line profiles. The properties of CO(2–1) line profiles for each shock model are shown in Table 4. We generated a priori C-shock models with pre-shock density \(5 \times 10^3 < n(H_2) < 2 \times 10^4 \) cm\(^{-3}\), shock velocity 50 and 50 km s\(^{-1}\), dimensionless magnetic factor \(b = B(n_{H_2})^{-1/2} \approx 2.5, 2.8 \mu G \text{ cm}^{-1.5}\), and shock ages estimates from 5000–10000 yr. Line profile calculations will require separate post-processing, which is discussed in detail in Section 4.

Besides the key shock properties mentioned in the previous paragraph, we used the following for all models. The cosmic-ray ionization rate \(\zeta\) is chosen to be \(2 \times 10^{−15} \) s\(^{-1}\) based upon elevated cosmic-ray rates measured near IC 443 (Indriolo et al. 2010). The initial conditions of the gas were adopted from those of a steady-state photodissociation region model for gas density \(2 \times 10^3 \) cm\(^{-3}\), solar-circle interstellar radiation field, and low extinction (\(A_V = 0.1\)). These pre-shock conditions result in a temperature of 47 K, which is higher than a nominal, quiescent molecular cloud, far from the supernova. The thickness of the shocked layer depends upon the temperature and chemical state of the pre-shock gas, which may not be well known. For this work, we use the high cosmic-ray ionization rate measured specifically in the molecular gas near IC 443.

The Paris–Durham shock models can readily predict the brightness of atomic lines, such as those of the neutral oxygen [OI] and the singly ionized carbon atom [CII]. They are included as additional shock diagnostics specifically for the W28 BML4 observations, as C and O data are available.

\(^{1}\) https://ism.obspm.fr/shock.html

### Table 4

| No. | \(n(H_2)\) (cm\(^{-3}\)) | \(V_{\text{shock}}\) (km s\(^{-1}\)) | \(b\) (\(\mu G \text{ cm}^{-1.5}\)) | Age (yr) | \([\text{CII}/\text{O}]\) | Pre-shock Cut (1 \(
\times \) 10\(^4\) cm\(^{-1}\)) | Post-shock Cut (1 \(
\times \) 10\(^5\) cm\(^{-1}\)) | FHWM (km s\(^{-1}\)) | \(\int T_dV\) (K km s\(^{-1}\)) |
|-----|-----------------|-----------------|-----------------|--------|-----------------|-----------------|-----------------|-----------------|-----------------|
| (1) | 20,000 | 50 | 2.8 | 5000 | 0.1 | 3–6 | 2 | 19.40 | 7.71 |
| (2) | 10,000 | 50 | 2.8 | 5000 | 7 | 5–8 | 2 | 22.07 | 6.5 |
| (3) | 35 | 2.5 | 5000 | 6 | 8–20 | 5 | 16.05 | 10.38 |
| (4) | 5000 | 35 | 2.8 | 5000 | 50 | 9–20 | 10 | 14.72 | 0.84 |

**Note.** Densities and shock velocities are chosen based on prior works (van Dishoeck et al. 1993; Reach et al. 2019) and serve as baselines for the demonstration of the theoretical model, as opposed to precision measurement. The integrated intensity of CO emission from each shock model is included as a sanity check with observation, on the basis that scale factors from 0.1–2 are reasonable. Also included are the properties of the prediction: the LVG integration range and the FHWM.

4. **Predictions of Velocity Distribution of CO in W28 and IC 443**

#### 4.1. Large Velocity Gradient Approximation

In this work, we have made use of the large velocity gradient (LVG) approximation introduced by Sobolev (1957). In an expanding shell, such as in an SNR, if the Doppler shift due to the velocity gradient between gas cells is larger than the local thermal line width, a photon may find itself *escaping* absorption (Sobolev 1957; Surdej 1977; Hummer & Rybicki 1985).

To solve the radiative transfer equation, we first find the coefficients for emission and absorption, which depend on the level population of each line. The level population \(n\) (per cubic centimeter) is derived from the *on-the-spot* assumption that incoming and outgoing transitions from each energy level are balanced while the gas is at the same spatial location. Moreover, with the use of the LVG approximation, the probability that photons might escape absorption is represented by \(\beta_i\) for transition \(i \rightarrow j\). The population balance equation is determined by

\[
\beta_{i+1,j} n_i A_{i+1,j} + (n_i + 1) B_{i+1,j} - n_i B_{i,j} + \sum_{k \neq j} (n_k C_{k,i} - n_i C_{i,k})] = 0, \tag{1}
\]

where \(A\) and \(B\) are the Einstein rate coefficients for spontaneous and stimulated emission, and \(C\) is the collisional rate coefficient for transitions at given temperatures obtained from laboratory measurements; we obtained the collisional and radiative...
transition rates from LAMDA\(^5\). \(I_\nu\) is the Planck function \((2\hbar\nu^3/c^2)/(h\nu/kT−1)\) evaluated at the background temperature \(T_{\text{CMB}} = 2.73\) K, which dominates at microwave frequencies (Gusdorf et al. 2008a, Section A.3 therein).

An approximation for the escape probability is given by Neufeld & Kaufman (1993) as \(\beta_{ij} = [1 − \exp(−[3\tau_{ij}])] / [3\tau_{ij}]\). The radiation field can be approximated by \(\bar{J}_\nu = S_{ij}(1 − \beta_{ij}) + \beta_{ij}I_\nu\), where \(S_{ij} = j_\nu / \alpha_{\nu}\) is the source function.

The escape probability approximation neglects radiative energy transport from one part of the medium to the next. By combining the single-point level population from the escape probability method with a simple first-order Olson & Kunasz (1987, denoted OK87) numerical scheme (see Equation (7)), a line profile could be modeled by finding \(I_\nu\) for each value of \(v_\nu\). Past work by Gusdorf et al. (2008a) in creating fast FORTRAN routines has provided computationally inexpensive, grid-based calculation of the population of CO up to \(J = 41\). In Figure 4, we compare the line intensities derived in this work with the LVG approximation with the well-used RADEX code of van der Tak et al. (2007).

4.2. Radiative Transfer

Radiative transfer within gases is dominated by emission and absorption lines. For the line transfer, the emission and extinction coefficient for a transition \(i \rightarrow j\) are given by the level population, \(n\): \[ j_{\nu,i} = \frac{h\nu_i}{4\pi} n_i \mu_i \phi_i(\nu), \] and \[ \alpha_{\nu,i} = \frac{h\nu_i}{4\pi} (n_j \mu_j - n_i \mu_i) \phi_j(\nu), \] where \(A_{ij}\) and \(B_{ij}\) are the Einstein coefficients for spontaneous and stimulated emission. They are related such that \(A_{ij} = \frac{2\hbar \nu_j}{c^2} B_{ij}\) (s\(^{-1}\)) and \(g_j B_{ij} = g_i B_{ji}\), where \(g\) is the statistical weight of a given level.

The photon that is emitted or absorbed may not be exactly at the same frequency \(\nu\), due to many broadening effects. The line broadening function \(\phi(\nu)\), the probability that a photon from a given transition is observed at frequency \(\nu\), is such that \[ \int_{0}^{\infty} \phi(\nu) d\nu = 1. \] In shock, the broadening of emission lines is due to effects such as the Doppler shift, due to various velocity components in the shock region and the inclination with respect to the line of sight. In this work, all the velocity components sum as an observer-frame velocity \(v_{\text{obs}}\), such that the broadening function \(\phi(\nu)\) is given by

\[ \phi(\nu) = \frac{\lambda_s}{\sqrt{2\pi} \sigma} \exp \left[ -\frac{(v_{\text{obs}} \cos \theta - \nu)^2}{2\sigma^2} \right], \]  

where \(v_{\text{obs}} = v_{\text{gas}}(z) - v_{\text{shock}} - v_{\text{preshock}}\) (the velocities are gas parcel velocity at position \(z\); shock velocity in the shock frame; and the ambient velocity in the pre-shock environment, respectively). The angle \(\theta\) is from the line of sight to the shock normal. The shock-frame gas velocity \(v_{\text{gas}}\) at position \(z\) is given by the neutral gas evolution in the shock model, whereas the shock and pre-shock velocity are fitting parameters. The line width due to thermal velocity is given by 3D Planck thermal dispersion \(\sigma = (8kT/\pi \mu \mu_{\text{H}})\), where \(\mu\) is the molecular mass in atomic mass units.

Finally, then, the rate of change of the specific intensity \(I_\nu\) (erg cm\(^{-1}\) s\(^{-1}\) sr\(^{-1}\) Hz\(^{-1}\)) along the line of sight \(s\) can be found. Radiative transfer in a medium is described by an ordinary differential equation:

\[ \frac{dI_\nu}{ds} = j_\nu - \alpha_{\nu} I_\nu. \]  

For optically thin cases, the absorption coefficient can be discarded. The intensity then is found simply by integrating the emission coefficient over the distance \(z\), projected as \(z = s \cdot \cos(\theta)\):

\[ I_\nu = \int_{z_i}^{z_f} j_\nu dz. \]  

More complex numerical integration methods are employed for an optically thick transition. The first-order, \(\tau\)-grid method from OK87 assumes that the source function \(S_{ij} = j_\nu / \alpha_{\nu}\) stays constant within a cell, but can change from cell to cell. If we integrate along the direction \(z\) normal to the parallel planes, the intensity is

\[ I_{i+1/2} = e^{-\Delta \tau} I_{i-1/2} + (1 - e^{-\Delta \tau}) S_{i-1/2}, \]  

where

\[ \Delta \tau = (z_{i+1/2} - z_{i-1/2}) \frac{\alpha_{\nu}}{\cos(\theta)}. \]  

For the second-order OK87 solution, the source function may vary linearly within the cell. In this case, the intensity is

\[ I_{i+1/2} = e^{-\Delta \tau} I_{i-1/2} + Q_{i}. \]  

\(^5\) https://home.strw.leidenuniv.nl/~moldata/
In this work, we use the LVG approximation to predict the line profile of CO transitions. Our approximation is valid only when the velocity gradient in a characteristic length \( L \) is much greater than the local thermal velocity gradient within it as

\[
\left| \frac{dV_n}{dz} \right| \gg \frac{V_{\text{th}}}{L},
\]

where \( L = T_n/(dT_n/dz) \). In Figure 5, we compare the gradient of the gas velocity \( (dV_n/dz) \) with that of the thermal velocity \( V_{\text{th}}/L \). One can see that the velocity gradient is sufficient such that LVG is satisfied only within a certain location of \( z \) in the shock. Beyond this distance, the LVG condition failed, and our
scheme is invalid. Thus, we stop integrating Equation (9) when \( \frac{n_L}{L} \leq \frac{\nu_{th}}{L} \).

As an example, Figure 6 compares the line profiles produced when integrating the entire shock region and plane-parallel slabs. Integration into the invalid LVG condition pronounces erroneous and nonthermal profiles. The generation of correct line profile prediction thus depends heavily on the consideration of a suitable integration range. In this case, the integration range is limited to roughly \( z \sim 10^{16} \) cm.

### 5. Result of Line Profile Fits

#### 5.1. Line Profile Fits for W28

Generally, we found that previous estimates (by excitation diagrams and emission-line diagnostics) of shock properties for each observation agrees with the prediction from CO observations. The agreement between different post-processing methods—prediction of CO line profile and estimates from excitation diagram—shows strong pre-shock density and thus the magnetic field strength.

Due to the 1D nature of the method, however, there is room for a mismatch. It is possible to attribute a two-component, two-shock-velocity model using an excitation diagram to an observation that is a single component with a large shock velocity (van Dishoeck et al. 1993). In our case, our model is only tuned to the molecular shock and we tried to find spec dominated by a single shock to test the theoretical model, as our single shock model best reproduces the line width of the observation.

Absolute brightness depends on other detailed precision parameters (beam filling factors, etc.) that are unknown. We do not account for absolute brightness with this theoretical demonstration, only the profile line width as it directly constrains shock velocity. Thus, the maximum brightness intensity is set to 1. The integrated intensity of line profile (\( \int \Gamma dV \)) from each observation and each model is included in Tables 2–4, which serves as a sanity check for choosing which model fits the observation, on the basis that scale factors from 0.1–2 are reasonable.

From the a priori shock models in Table 4, we produced line profile fits for the observations summarized in Table 5. Further constraints from molecular lines ratio are used when available. For the high-J CO(16–15) observation of W28 BML4 (Figure 7), the line width limits the shock velocity to \( V_{\text{shock}} \sim 50 \) km s\(^{-1}\). A key constraint is the ratio \( \langle \text{C II} \rangle / \langle \text{O I} \rangle \sim 5 \). Both the \( n(\text{H}_2) \sim 10^4 \) and \( 5 \times 10^3 \) cm\(^{-3}\) models match the line width, but from Table 4, the latter produces a \( \langle \text{C II} \rangle / \langle \text{O I} \rangle \) ratio.
10 times larger than the observation. It is more likely that the emission originates from shock into denser gas at 10^4 cm^−3.

We found that the same model can reproduce the CO (2–1) observation from Reach et al. (2005) in the BML4 region. The emission, though, appears to be reversed in the direction inferred from its central velocity. The absorption feature at +5 km s^−1 (FWHM = 1.2 km s^−1) infers the velocity of unshocked, cold, ambient gas.

5.2. Line Profile Fits for IC 443

We follow the same roadmap for the prediction of the CO line profile with IC 443. Excitation models were used to estimate shock properties in both observations of van Dishoeck et al. (1993) and Rho et al. (2021). Reach et al. (2019) have developed a theoretical line profile prediction for H2 from various observations of IC 443 B, C, and G, which will serve as a useful shock diagnostic. Line profile modeling of near-infrared emission H2 S(5) with SOFIA from Reach et al. (2019) provided constraints on a pre-shock density of n(H2) ≃ 10^7−10^8 cm^−3, and a shock velocity in the range of 30–60 km s^−1, sufficient to produce the observed H2 line widths.

The CO observation of van Dishoeck et al. (1993) provided exhaustive constraints on the origin of the CO emission in IC 443. From the ^12CO and ^13CO line ratios and excitation calculation for clumps B and C, the best fits of the excitation calculation indicate a pre-shock density of n(H2) ≃ 10^7−10^8 at an initial gas temperature of less than 20K. Quite importantly, the pre-shock density of clump G cannot exceed 5 × 10^3 cm^−3, due to self-absorption of HCO^+ and HCN, indicating a low excitation temperature (Section 5.2 of van Dishoeck et al. 1993).

In this work, we found the line width from a priori models sufficient to reproduce observations in clump GI. For both CO (2–1) and CO (3–2), one-component models n(H2) ≃ 8 × 10^3 cm^−3 and V_shock ≃ 35 km s^−1 make good fits to the observation (see Figure 8). This prediction is in agreement with the prediction from the H2 theoretical modeling of Reach et al. (2019) (6 × 10^3 cm^−3, 37 km s^−1) and infers that denser, high-frequency CS producing components (∼10^5 cm^−3) are well separated from the low-J CO producing component in this region, a conclusion reflected both in Turner (1992) and van Dishoeck et al. (1993), where lower-density gas is suggested to be responsible for the low-frequency emission of CO (e.g., (3–2) and (2–1)), and the higher density for high-frequency CS, (e.g., (5–4) and (7–6)). The strong self-absorption feature of both CO (2–1) and CO (3–2) in the clump GI, around −5 km s^−1, suggests the ambient gas velocity.
However, it should be noted that observations of other clumps of IC 443 from van Dishoeck et al. (1993) are explained with a two-component model, with a line width up to \( \sim 80 \, \text{km} \, \text{s}^{-1} \) for which slow C-shock models alone cannot reproduce. Shock fits of \( n(H_2) \sim 10^4 \, \text{cm}^{-3} \) and \( V_{\text{shock}} \sim 35 \, \text{km} \, \text{s}^{-1} \) were made for the CO(2–1) observation of the H3 position from Rho et al. (2001). This prediction is in agreement with the H\(_2\) line data and excitation models of Rho et al. (2001) and Cesarsky et al. (1999), suggesting fast J shock \( (n(H_2) < 10^3 \, \text{cm}^{-3}, V_{\text{shock}} \) up to 100 km s\(^{-1}\)) and slow C shock \( (n(H_2) \sim 10^3 \, \text{cm}^{-3}, V_{\text{shock}} \) up to 50 km s\(^{-1}\)) (McKee & Draine 1991, Figure 2) through a dense medium with varying density, in which denser, non-dissociative CO gas mostly probe for slow C shocks.

6. Conclusion

The development of line profile prediction directly from shock models would strengthen many links in the studies of SNR–molecular cloud interaction. Shocks are ubiquitous major drivers of star formation, sources of cosmic-ray acceleration, and sculptors of filamentary magnetic field structure. From the Paris–Durham MHD 1D shock model, constraints such as pre-shock density, shock velocity, B-field strength, and cosmic ionization rates are all available as shock diagnostics for related studies.

We presented a post-processing framework to produce the theoretical line profiles of pure rotational emission of CO from the Paris–Durham shock model. This is done by considering the LV approximation and the effect of optically thick plane-parallel slabs in the integration range of the 1D model.

We found that rotational emissions of CO are mainly generated in the rapid cooling phase of shock. In comparison to H\(_2\) emission lines, CO emits much later in the shock frame than H\(_2\), due to its lower excitation energy.

We tested the framework on CO(16–15), CO(11–10), CO(3–2), and CO(2–1) observations in regions BML4 and OH(1) of SNR W28 for a shock velocity of 50 km s\(^{-1}\) and pre-shock density of \(10^4 \, \text{cm}^{-3}\), finding the prediction well represented by the shock studies of Reach et al. (2005) and Gusdorf et al. (2012).

We also modeled CO line profiles for CO(3–2) and CO(2–1) in the clump GI and H of SNR IC 443 with shock velocity of 35 km s\(^{-1}\) and pre-shock density of \(8 \times 10^3-10^4 \, \text{cm}^{-3}\). The prediction is in close agreement with the excitation models from van Dishoeck et al. (1993) and Rho et al. (2001), and also in agreement with H\(_2\) theoretical modeling from Reach et al. (2019).

We showed that the CO line profile prediction provides robust constraints on the shock velocity and becomes an additional valuable tool for probing shocks into molecular clouds. Our proposed scheme can directly be extended to other molecular lines of interest, such as SiO.

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