A PHOTON-DOMINATED REGION MODEL FOR THE FIR MID-J CO LADDER WITH UNIVERSAL ROTATIONAL TEMPERATURE IN STAR FORMING REGIONS

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ABSTRACT

A photon-dominated region (PDR) is one of the leading candidate mechanisms for the origin of warm CO gas with near universal \( \sim 300 \) K rotational temperature inferred from the CO emission detected toward embedded protostars by Herschel/PACS. We have developed a PDR model in general coordinates, where we can use the most adequate coordinate system for an embedded protostar having outflow cavity walls, to solve chemistry and gas energetics self-consistently for given UV radiation fields with different spectral shapes. Simple one-dimensional tests and applications show that FIR mid-\( J \) (\( 14 \leq J \leq 24 \)) CO lines are emitted from close to the surface of a dense region exposed to high UV fluxes. We apply our model to HH46 and find that the UV-heated outflow cavity wall can reproduce the mid-\( J \) CO transitions observed by Herschel/PACS. A model with UV radiation corresponding to a blackbody of 10,000 K results in a rotational temperature lower than 300 K. The results of these models therefore spread out up to 1 dex in the predicted thermal structure in the far-ultraviolet (FUV) irradiated gas.

Most PDR models have concentrated on bright, dense, quiescent molecular gas exposed to radiation from O stars. However, FUV observations and theoretical models of classical T-Tauri stars show that these sources emit FUV radiation approximated by a 10^4 K blackbody radiation (hereafter BB1.0) produced mostly by accretion (e.g., Gullbring et al. 1998; Calvet et al. 1998; Johns-Krull et al. 2000; Yang et al. 2012). This FUV spectrum with a lower effective temperature than those of O stars affects the composition and structure of PDRs (Spaans et al. 1994) because the reduction in the FUV radiation at the shortest wavelengths (912–1100 Å) reduces the efficiency of the photoelectric heating on polycyclic aromatic hydrocarbons (PAHs) and small dust grains (Spaans et al. 1994), and also reduces the photodissociation rates of H₂ and CO (van Dishoeck et al. 2006).

The PDR model for the embedded protostar with outflow cavity walls must deal with a system that is at least two-dimensional (2D) and to cover a high dynamic range of physical parameters at radii from \( \sim 10 \) AU to \( \sim 10^4 \) AU. Recently, some PDR models have begun to consider the requisite 2D geometries (e.g., van Zadelhoff et al. 2003; Bruderer et al. 2009a; Woitke et al. 2009). These 2D PDR models use the cylindrical coordinate system concentrating on the protoplanetary disk. However, the cylindrical coordinate system requires a large number of grids, and thus increases the computational time to model the outflow cavity walls of embedded protostars with a reasonable spatial resolution. For example, Bruderer et al. (2009a) modeled the UV heated outflow cavity walls with \( \sim 10^5 \) grid cells.

In this paper, we apply a new PDR code to the 2D density structure of embedded outflow sources combined with a 15,000 K blackbody FUV radiation field (hereafter BB1.5), fitted to the observed UV spectrum of TW Hya (e.g., Herczeg et al. 2002; Yang et al. 2012), as well as BB1.0 and the Draine field.

1. INTRODUCTION

Many energetic phenomena, such as high-energy photons produced from accretion onto a protostar and jets ejected from the star–disk boundary region, affect the physical and chemical structures of the disk and envelope simultaneously. This material is heated to a temperature from \( \sim 100 \) to \( \sim 1000 \) K, where many key gas coolants are excited to emit in the far-infrared (FIR); in this respect, CO is one of the most important coolants.

Low-mass embedded protostars were observed with the Long Wavelength Spectrometer (Clegg et al. 1996) on board the Infrared Space Observatory (ISO, e.g., Benedettini et al. 2003; van Dishoeck 2004). The CO rotational temperature \( T_{\text{rot}} \) obtained by fitting the CO excitation diagrams (up to \( J = 19–18 \), \( E_{\text{up}} = 1050 \) K) were a few hundred to \( \sim 1000 \) K. Because of the low spatial resolution of ISO, however, the heating mechanism of CO gas (high-energy photons or shocks) was not well constrained.

More recently, observations of embedded low-mass protostars with the Photodetector Array Camera and Spectrometer (PACS; Poglitsch et al. 2010) on board the Herschel Space Observatory (Herschel) revealed two temperature (warm and hot) CO gas components (Manoj et al. 2013; Karska et al. 2013; Green et al. 2013), which may be attributed to a photon-dominated region (PDR) and shock, respectively. Visser et al. (2012) showed that the warm component of CO gas with \( T_{\text{rot}} \sim 300 \) K can be produced by the PDR along the outflow cavity walls combined with a C-shock by modeling the CO fluxes detected with PACS. Visser et al. (2012) also showed that the contribution of PDR to the CO emission increases with evolution.

Many theoretical PDR models have been developed over the past three decades (e.g., Röllig et al. 2007, hereafter R07). Some codes deal with the detailed microphysics needed to model both chemistry and thermal balance (e.g., Le Petit et al. 2006, 2009), while others use approximate formulae or a reduced chemical network (e.g., Röllig et al. 2006; Bruderer et al. 2009a; Woitke et al. 2009). The results of these models therefore spread out up to 1 dex in the predicted thermal structure in the far-ultraviolet (FUV) irradiated gas.
propagation direction. When a photon propagates as much as \( ds \), a trajectory of the photon is described in the Cartesian coordinate as

\[
\vec{X} = \vec{X}_0 + \vec{\delta} \cdot ds
\]

\[
(x, y, z) = (x_0, y_0, z_0) + (\delta_x, \delta_y, \delta_z) \cdot ds,
\]

where \( \vec{X}_0 \) is the current position, \( \vec{X} \) is the next position, and \( \vec{\delta} \) is the direction vector. Because the surface of the grid can be described by a simple equation with \( x, y, \) and \( z \) in the Cartesian coordinates, we can find \( ds \) by solving the equation of the photon trajectory intersecting the surface of the grid in any coordinate system.

For example, the boundary between the outflow cavity and the envelope can be described by

\[
z = \delta_0 \times (x^2 + y^2)
\]

\[
= \left( \frac{1}{10^6 \text{AU} \tan^2(\alpha/2)} \right) \times (x^2 + y^2),
\]

where \( z \) is the outflow axis and \( \alpha \) is the full opening angle at \( z = 10^6 \text{AU} \) (Bruderer et al. 2009a). As the boundary parameter \( \delta_0 \) describes a circular paraboloid, the circular paraboloid with \( \delta \equiv z/(x^2 + y^2) \) can be used as a new coordinate instead of a circular conical surface \( \theta \) in the spherical coordinates. In this \( (r, \delta) \) coordinates, using Equation (1) and the definition of \( \delta \), we find the quadratic equation of the photon trajectory intersecting the \( \delta \) surface as

\[
A \cdot ds^2 + B \cdot ds + C = 0,
\]

where

\[
A = \delta(\delta^2 + \hat{y}^2)
\]

\[
B = 2\delta(\delta x_0 + \hat{y}y_0) - \hat{z}
\]

\[
C = \delta(\delta^2 + \hat{y}^2) - \hat{z}^2.
\]

Therefore, in order to minimize the computational time, we can choose a coordinate system optimized for a given physical model, which can provide enough spatial resolution with a relatively small number of grids (see Section 5 for more details).

2.2. FUV Radiative Transfer

The FUV radiative transfer is calculated by the method of van Zadelhoff et al. (2003) and Bruderer et al. (2009a). We calculate the FUV radiative transfer at only one representative wavelength where photon energy is 9.8 eV (the middle of the 6–13.6 eV FUV band) and then measure the FUV strength (the unattenuated FUV strength \( G_0 \) and average visual extinction \( A_\lambda \)) of the integrated intensity from 912 to 2050 Å as ISRF, 1 cm\(^{-2}\) erg cm\(^{-2}\) s\(^{-1}\) (Habing 1968). Therefore, BB1.0 and BB1.5 are normalized to have the same integrated intensity from 912 to 2050 Å as ISRF, and the Draine field (\( \chi \), Draine 1978) is given by \( \chi = G_{\text{dust}}/1.71 \). We adopt dust properties for the average Milky Way dust in molecular clouds with \( R_V = 5.5 \) and C/H = 48 ppm in PAHs (Draine 2003) for this calculation.

To derive the unattenuated FUV strength \( G_0 \) and the attenuated FUV strength \( G_{\text{dust}} \) in the 2D space, we solve the FUV radiative transfer with the dust scattering using the Heneyey-Greenstein phase function

\[
P(\cos \phi, g_\lambda) = \frac{1 - g^2_\lambda}{4\pi[1 + 2g^2_\lambda - 2g_\lambda \cos \phi]^{3/2}}
\]
with the mean scattering angle \( g_s = \langle \cos \phi \rangle = 0.767 \). The scattering optical depth is first calculated using random number \( \xi \) between 0 and 1 as

\[
\tau_{\text{scat}} = -\ln(1 - \xi),
\]

which can be converted to an absorption optical depth,

\[
\tau_{\text{abs}} = \tau_{\text{scat}} \times \omega/(1 - \omega)
\]

with the dust grain albedo \( \omega = 0.387 \).

Each model photon has the initial intensity \( I(0) \) given by

\[
I(0) = \frac{F \cdot S}{N_{\text{phot}}},
\]

where \( F \) is the flux entering the system, \( S \) is the total surface that the photon passes through, and \( N_{\text{phot}} \) is the number of model photons. The model photon propagates until it reaches the optical depth \( \langle \tau_{\text{scat}} \rangle \) at which it scatters, and its intensity drops according to

\[
I_i(s + \Delta s) = I_i(s) \exp(-\Delta \tau_{\text{abs}}),
\]

where \( \tau_{\text{abs}} = (1 - \omega) C_{\text{ext}} n \Delta s \),

\[
C_{\text{ext}} \text{ is an extinction cross section of } 1.075 \times 10^{-21} \text{ cm}^2 \text{ per H nucleus, } n(= n_H + 2n_{H_2}) \text{ is the total hydrogen number density, and } \Delta s \text{ is the path length traveled within a grid cell. Therefore, the dust attenuated FUV strength } G_{\text{dust}} \text{ in a grid cell with the volume } V
\]

\[
G_{\text{dust}} = \frac{1}{1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ V}} \sum I_i \Delta s \frac{1 - \exp(-\Delta \tau_{\text{abs}})}{\Delta \tau_{\text{abs}}},
\]

where the sum is taken over all photon packages passing the grid cell. The unattenuated FUV strength \( G_0 \) in the grid cell with the volume \( V \) is

\[
G_0 = \frac{1}{1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ V}} \sum I_0 \Delta s,
\]

and the average visual extinction \( \langle A_V \rangle \) is

\[
\langle A_V \rangle = -\ln \left( \frac{G_{\text{dust}}}{G_0} \right) \frac{1}{2.5 \log(e)} k_{UV/V},
\]

where the conversion factor of \( k_{UV/V} (= A_{UV}/A_V) \) is 1.6. As each photon passing the grid cell comes through a different column density, \( \langle A_V \rangle \) is the mean over all photons. \( A_V \) is the visual extinction in the one-dimensional (1D) model and related directly to the column density while \( \langle A_V \rangle \) is calculated with Equation (12) in the 2D model and averaged over all photons. We note that \( G_0 \) is calculated by neglecting absorption by dust grains, i.e., scattering by grains is still considered. Otherwise, \( G_{\text{dust}} \) is larger than \( G_0 \) in some cases, resulting in a negative value of \( \langle A_V \rangle \). To prevent this effect, we define \( G_0 \) as a FUV strength in the absence of only absorption by grains, following Bruderer et al. (2009a).

For the convergence, the number of model photons is doubled until the difference in \( G_{\text{dust}} \) in two consecutive steps, \( |G_{\text{dust}}(\text{previous}) - G_{\text{dust}}(\text{current})|/G_{\text{dust}}(\text{current}) \), is smaller than 5% for all grid cells where \( G_{\text{dust}} \) is larger than \( 10^{-4} \) ISRF.

### 2.3. Chemistry

For chemistry, we have modified the Heidelberg “ALCHEMY” code (Semenov et al. 2010). The basic equations for species in the gas phase (\( n(i) \)) are described as

\[
\frac{dn(i)}{dt} = -n(i) \sum n(j) k_{ij}^{g2} + \sum n(j) n(k) k_{jk}^{g2} - n(i) k_{i}\text{ad} + n_i(k) k_{i}\text{des}.
\]

In this equation, the first term indicates the destruction process of the given species \( n(i) \) by reacting with another species, and the second term describes the formation process by the reactions of the two other species. The third and fourth terms represent the destruction and formation of the species, respectively, through photodissociation/ionization and cosmic ray ionization. The last two terms describe the adsorption and desorption of the species onto and out of grain surfaces, respectively.

The gas-phase chemical reaction network is based on the UMIST2006 database (Woodall et al. 2007) modified by Bruderer et al. (2009b). The two-body reaction rate is expressed as

\[
k_{g2} = \alpha_{g2} \times \left( \frac{T_{\text{gas}}}{300 \text{ K}} \right)^{\beta_{g2}} \exp(-\gamma_{g2}/T_{\text{gas}}) \text{ cm}^3 \text{ s}^{-1},
\]

where \( \alpha_{g2}, \beta_{g2}, \) and \( \gamma_{g2} \) are coefficients that depend on reaction types.

The FUV photoreaction rate is described as

\[
k_{\text{ph}} = \chi \alpha_{\text{ph}} \exp(-\gamma_{\text{ph}} A_V) \text{ s}^{-1},
\]

where \( \chi \) is the FUV strength in the Draine field. Unshielded rates (\( \alpha_{\text{ph}} \)) are calculated with the cross sections given by van Dishoeck et al. (2006), and dust attenuation factors, \( \gamma_{\text{ph}} \) for \( R_V = 5.5 \) grain, are adjusted by the method of Röllig et al. (2013). Unshielded photo-dissociation rates of H2 and CO in BB1.0 are \( 3.16 \times 10^{-12} \text{ s}^{-1} \) and \( 1.90 \times 10^{-11} \text{ s}^{-1} \), respectively, which are an order of magnitude lower than the rates in the Draine field because the intensity between 912 and 1100 Å in BB1.0 is an order of magnitude lower than that of the Draine field (van Dishoeck et al. 2006).

Self-shielding of H2 and CO cause the rapid decrease of their photodissociation. The approximate formula for the H2 self-shielding is given by

\[
\beta_{H2} = 0.965 \times \left( 1 + \frac{x_{H2}/b_5}{5} \right)^0.035 + \exp[-8.5 \times 10^{-4}(1 + x_{H2})^{0.5}],
\]

where \( x_{H2} = N_{H2}/5 \times 10^{14} \text{ cm}^{-2} \) and \( b_5 \equiv b/10^5 \text{ cm}^{-1} \) (Draine & Bertoldi 1996). Here, \( N_{H2} \) is the H2 column density and \( b \) is the Doppler broadening parameter (\( b \equiv \text{FWHM}/\sqrt{4ln2} \)), which is assumed to be 1.1 km s\(^{-1}\). For the CO self-shielding effect, we interpolate the values in Table 6 (b(CO) = 0.3 km s\(^{-1}\), \( T_C \text{CO} = 50 \text{ K} \) in Visser et al. (2009). Neutral carbon is also shielded by H2 in addition to the self-shielding, which is taken into account by a simple factor (Kamp & Bertoldi 2000; Woitke et al. 2009):

\[
\beta_{C} = \exp \left( -\sigma_{C} \frac{N_{C}}{N_{\text{IC}}} - 0.97 \frac{T_{\text{IC}}^{0.27}}{10^{22} \text{ cm}^{-2}} \left( \frac{N_{H2}}{10^{22} \text{ cm}^{-2}} \right)^{0.45} \right),
\]

\( N_{\text{IC}} \) is the total surface density of IC.
with the neutral carbon column density, $N_C$ and the FUV-averaged cross section of the neutral carbon, $\sigma_C^{bf} = 1.1 \times 10^{-17}$ cm$^2$.

In a deeper region of the PDR, where most FUV photons are shielded, the cosmic ray significantly affects the chemistry. The cosmic-ray desorption rate is calculated using the formalism of Hasegawa & Herbst (1993).

$$k_{crd} = f(70\, K) \, k_{ad}(70\, K) \, \frac{\zeta_{\text{CR}}}{5.0 \times 10^{-17} \, \text{s}^{-1}}$$

where $k_{ad}(70\, K)$ is the thermal desorption rate at 70 K and $f(70\, K)$ is the ratio of the grain cooling timescale via desorption of species to the timescale of subsequent heating events. We adopt $f(70\, K)$ as $3.16 \times 10^{-19}$ for the grain size of $0.1\, \mu m$ from Hasegawa & Herbst (1993).

The photodesorption rate by UV photons is calculated following the method of Woitke et al. (2009):

$$k_{phd} = \frac{n_{gr}}{N_p} \times n_{act} Y G_{dust} F_D \, s^{-1} \quad \text{if} \quad N_m < N_p$$

$$= \frac{n_{gr}}{n_{ice}} \times Y G_{dust} F_D \, s^{-1} \quad \text{if} \quad N_m \geq N_p,$$

where $n_{act}$ ($= 4\pi a_{gr}^2 N_s n_{gr}$) is the number of active surface sites in a monolayer of ice on per volume, $n_{ice} = \sum_j n_j(j)$ is the total number of ice species, and $Y$ is the photodesorption yield (the number of ice species ejected per incident photon). $F_D$ is the conversion factor of $G_{dust}$ to the photon number flux, which is $1.93 \times 10^6 \, \text{cm}^{-2} \, \text{s}^{-1}$ for the Draine field and $2.33 \times 10^9 \, \text{cm}^{-2} \, \text{s}^{-1}$ for BB1.0. $N_m = n_{ice}/n_{act}$ is the number of monolayers. We assume $N_p = 2$ because the photodesorption by UV photons occurs in the upper $\sim 2$ monolayers (Oberg et al. 2007).

We follow the model of H$_2$ formation on interstellar dust grains via physisorption and chemisorption from Cazaux & Tielens (2002, 2004, 2010).

$$k_{\text{H}_2} = \frac{1}{2} n_H v_H n_{gr} \sigma_{gr} \epsilon_{H_2} S_H \, \text{cm}^3 \, \text{s}^{-1},$$

where $n_H$ and $v_H$ ($= 1.45 \times 10^4 \sqrt{T_{\text{gas}}}$ cm s$^{-1}$) are the number density and thermal velocity of H atoms in the gas phase, and $S_H$ is the sticking coefficient of the H atoms (Hollenbach & McKee 1979),

$$S_H = 1 + 0.04 \left( \frac{T_{\text{gas}} + T_{\text{dust}}}{100} \right)^{1/2} + 0.2 \frac{T_{\text{gas}}}{100} + 0.08 \left( \frac{T_{\text{gas}}}{100} \right)^{2}$$

The formation efficiency $\epsilon_{H_2}$ is given by Cazaux & Tielens (2002, 2004, 2010):

$$\epsilon_{H_2} = (A + 1 + B)^{-1} \xi$$

$$\epsilon_{H_2} = \left( \frac{\mu F}{2\beta_{H_2}} + 1 + \frac{\beta_{H_2}}{\alpha_{P}} \right)^{-1} \xi.$$
We set $A$ to zero to make newly formed H$_2$ molecules leave very cold dust surfaces, which is equivalent to the Equation (13) in Cazaux & Tielens (2002).

We include the electron attachment to grains and the recombination of cations with the negatively charged grains adopted from the Ohio State University Astrophysical Chemistry Group gas-phase database (Smith et al. 2004). The initial abundances in our model are listed in Table 2, which represent the molecular cloud abundances approximated from Aikawa & Herbst (1999).

| Species | Abundance $^a$ |
|---------|----------------|
| H$_2$   | 5.00E-1        |
| He      | 1.40E-1        |
| N       | 2.25E-5        |
| CN      | 6.00E-8        |
| H$_2$+  | 1.00E-8        |
| S$^+$   | 1.60E-6        |
| Si$^+$  | 1.60E-9        |
| Mg$^+$  | 3.00E-8        |
| Fe$^+$  | 2.00E-8        |
| H$_2$O(gr) | 2.50E-4 |
| GRAIN   | 6.00E-12       |

Note. $^a$ Abundance = ($n_X/n_\mathrm{H}$ + 2$n_{\mathrm{H}_2}$)), where $n_X$ is the number density of species $X$.

We use the constant value of $\Lambda_{\mathrm{RC}}/n_e$ at $\psi = 10^5$ K/cm$^3$ and $10^6$ K/cm$^3$ (see Röllig et al. 2013).

Spaan et al. (1994) calculated the photoelectric heating rate for the blackbody radiation field of an effective temperature ($T_{\mathrm{eff}}$). As photons below 6 eV also contribute the photoelectric heating, they used a modified unit, $G_{\mathrm{dust}}$ normalized to the Habing field to have the same integrated intensity from 2 eV to 13.6 eV. The heating rate can be calculated by multiplying Equation (28) (with $G_{\mathrm{dust}}$) by a simple correction factor, $e(T_{\mathrm{eff}})$.

$$
e(T_{\mathrm{eff}}) = \left( \frac{T_{\mathrm{eff}}}{30,000 \, \text{K}} \right) \times [\log(1.4 \times 10^{-4} \, \psi')]^{T_{\mathrm{eff}}}, \quad (30)$$

where $x(T_{\mathrm{eff}}) = -1$ if $T_{\mathrm{eff}} < 20,000$ K and $\psi' = (G_{\mathrm{dust}}T_{\mathrm{gas}}/n_e) > 2 \times 10^5$ K/cm$^3$, and 0 otherwise. In order to describe the photoelectric heating rate for a given $G_{\mathrm{dust}}$ normalized to the Habing field to have the same integrated intensity from 6 eV to 13.6 eV, $G_{\mathrm{dust}}$ is corrected as

$$G_{\mathrm{dust}} = G_{\mathrm{dust}} \int_{912}^{6196} \frac{B(B(30,000 \, \text{K})/x_{\psi} + 912 - 6196) d\lambda}{\int_{912}^{6196} B(B(30,000 \, \text{K})/x_{\psi} + 912 - 6196) d\lambda}, \quad (31)$$

where $B(B(30,000 \, \text{K})/x_{\psi})$ is the Planck function with $T_{\mathrm{eff}}$. The corrected unit, $G_{\mathrm{dust}} = 6.67G_{\mathrm{dust}}$, for the model of BB1.0 is used in Equations (28)–(30).

Figure 2 shows photoelectric heating efficiencies as functions of $\psi$ (in the unit of $G_{\mathrm{dust}}$) for given spectral types. Higher-energy (shorter wavelength) photons photoelectrically heat the gas more efficiently. For $\psi > 10^5$ K/cm$^3$, most grains are neutral and positively ionized, and only high-energy photons ($>$6 eV) can remove electrons from the grains. Therefore, the efficiency of the Draine field is higher than that of BB1.0.

However, for $\psi < 10^5$ K/cm$^3$, a large portion of a grain is negatively charged (see Figure 9 in Weingartner & Draine 2001a). As a result, photons with energies lower than 6 eV can remove electrons from the negatively charged grains, which have the first electron affinity lower than 6 eV (Bakes & Tielens 2001a).
The integrated intensity from 2 eV to 6 eV is larger than that from 6 eV to 13.6 eV by a factor of ∼6 for BB1.0, while most of the intensity is deposited above 6 eV for the Draine field. This results in a higher efficiency for BB1.0 than for the Draine field for a given heating rate from 2 eV to 6 eV is larger than that from 6 eV to 13.6 eV by a factor of ∼2.

**H₂ vibrational heating:** The gas is heated if a hydrogen molecule excited by FUV radiation is collisionally de-excited. Röllig et al. (2006) provides an approximated formula for the heating rate (Röllig et al. 2006) is

\[
\Gamma_{\text{H}_2} = n_{\text{H}_2} \frac{1.8 \times 10^{-11} k_{\text{ph}}}{1 + \left( \frac{1.9 \times 10^{-6} + 9.1 n_{\text{H}_2}}{\gamma_c n_{\text{H}_2}} \right)} \text{erg s}^{-1} \text{cm}^{-3},
\]

with the collision rate \(\gamma_c = 5.4 \times 10^{-13} \sqrt{T_{\text{gas}}} \text{cm}^{-3} \text{s}^{-1}\).

**H₂ formation heating:** If we assume that each H₂ formation process releases one-third of its binding energy to heat the gas, the corresponding heating rate (Röllig et al. 2006) is

\[
\Gamma_{\text{form}} = 2.4 \times 10^{-12} k_{\text{H}_2} n_{\text{H}} \text{erg s}^{-1} \text{cm}^{-3},
\]

where the \(k_{\text{H}_2}\) formation rate is described in Equation (25).

**H₂ dissociation heating:** About 10% of the radiative decays in the \(\text{H}_2\) dissociation deliver about 0.25 eV to the gas. This heating rate is taken from Meijerink & Spaans (2005),

\[
\Gamma_{\text{H}_2} = 2.63 \times 10^{-13} n_{\text{H}_2} k_{\text{ph}} \text{erg s}^{-1} \text{cm}^{-3}.
\]

We also slightly modify the equation with the local \(\text{H}_2\) photodissociation rate \(k_{\text{ph}}\).

**C ionization heating:** When a neutral carbon is ionized, a photo-electron released with the energy around 1 eV heats the gas (Woitek et al. 2009) with a rate of

\[
\Gamma_{\text{C}} = 1.602 \times 10^{-12} n_{\text{C}} k_{\text{ph}} \text{erg s}^{-1} \text{cm}^{-3},
\]

where \(n_{\text{C}}\) is the neutral carbon number density and \(k_{\text{ph}}\) is the local carbon photoionization rate corrected by the shielding factor in Equation (17).

**Cosmic ray heating:** For the low degree of ionization, \(<10^{-4}\), the primary ionization by a cosmic ray particle releases energy of about 9 eV to heat the gas. The heating rate is \(\Gamma_{\text{CR}} = 1.5 \times 10^{-13} \zeta_{\text{CR}} n \text{erg s}^{-1} \text{cm}^{-3}\).

**Fine structure line cooling:** The most prominent forbidden fine structure lines at the surface of outflow cavity walls are \([\text{O} i]\ 63 \mu\text{m}, \ [\text{O} i] 146 \mu\text{m}, \ [\text{C} i] 369 \mu\text{m}, \ [\text{C} i] 609 \mu\text{m}, \ [\text{Si} ii] 34.8 \mu\text{m}, \text{and} \ [\text{Si} ii] 158 \mu\text{m}\). We calculate the cooling rate using the escape probability method (e.g., Tielens 2005) and use the atomic and cationic data taken from the Leiden Atomic and Molecular Database (LAMBD db; Schöier et al. 2005) except for \(\text{Si}^+\) (Hollenbach & McKee 1979). The column densities of these species are assumed to be the products of the distance to the nearest boundary from the current grid and the local number densities of those.
**H$_2$ vibrational cooling:** Vibrational lines of H$_2$ can contribute to the cooling of the gas. Due to the large energy gap (6000 K) between the ground state and the first excited state, we use the two level approximation given in R"ollig et al. (2006),

\[
\Lambda_{\text{H}_2} = n \ n_{\text{H}_2} \ 9.1 \times 10^{-13} \ \gamma_c \ \exp(-6592 \ \text{K}/T_{\text{gas}}) \times \frac{8.6 \times 10^{-7} + 0.48 \ k_{\text{ph}}^{\text{H}_2}}{\gamma_c \ n + 8.6 \times 10^{-7} + 0.48 \ k_{\text{ph}}^{\text{H}_2}} \ \text{erg s}^{-1} \ \text{cm}^{-3} \]  

(36)

where $k_{\text{ph}}^{\text{H}_2}$ and $\gamma_c$ are described in Equation (32).

**Gas-grain cooling/heating:** The temperature difference between gas and dust leads to the transfer of heat. This can be an important coolant near the surface of the dense PDR where $T_{\text{dust}} < T_{\text{gas}}$. The rates are proportional to $T_{\text{dust}} - T_{\text{gas}}$. We adopt the results of Burke & Hollenbach (1983) with the dust cross section per H nucleus of $\sigma_d = 2.98 \times 10^{-21} \ \text{cm}^2$ (R"ollig et al. 2013),

\[
\Gamma_{\text{coll}} = 4.4 \times 10^{-33} n^2 \ \sqrt{T_{\text{gas}}} \left( \frac{\sigma_d}{2.98 \times 10^{-21} \ \text{cm}^2} \right) \times [1 - 0.8 \ \exp(-75/T_{\text{gas}})] (T_{\text{dust}} - T_{\text{gas}}) \ \text{erg s}^{-1} \ \text{cm}^{-3}. \]  

(37)

**Molecular cooling by CO and H$_2$O:** If CO and H$_2$O molecules exist, their lines can provide more efficient cooling than [O I] and [C II] lines. We calculate the molecular line cooling rate following the method of Meijerink & Spaans (2005) and Yan
Figure 6. Benchmarking results of V3 (left, log \( n \) = 5.5 and log \( \chi \) = 1) and V4 (right, log \( n \) = 5.5 and log \( \chi \) = 5).

(1997), which used the fitted cooling rate coefficients of Neufeld & Kaufman (1993) and Neufeld et al. (1995). Isotope ratios are assumed to be \(^{12}\text{C}/^{13}\text{C} = 69\) and \(^{16}\text{O}/^{18}\text{O} = 557\) (Wilson & Rood 1994). The column densities of CO and H\(_2\)O are calculated by the same methods as used for the column densities of atoms in the fine structure line cooling.

**Ly \( \alpha \) and OI-6300 Å cooling.** At a high gas temperature, Lyman \( \alpha \) and OI-6300 Å line cooling are important cooling processes. We adopt a simple approximated formulae from Sternberg & Dalgarno (1989):

\[
\Lambda_{\text{Ly} \alpha} = 7.3 \times 10^{-19} n_H n_e \exp(-118400/T_{\text{gas}}) \text{ erg s}^{-1} \text{ cm}^{-3}
\]

\( (38) \)

and

\[
\Lambda_{\text{OI-6300}} = 1.8 \times 10^{-24} n_O n_e \exp(-22800/T_{\text{gas}}) \text{ erg s}^{-1} \text{ cm}^{-3}
\]

\( (39) \)

with the atomic oxygen number density, \( n_O \).

**2.5. Line Radiative Transfer**

We have developed a new solver of a non-LTE line Radiative transfer In general Grid (RIG). RIG has been upgraded from RATRAN (Hogerheijde & van der Tak 2000) and use the same ray tracing method described in Section 2.1.

This code iteratively solves the equation of radiative transfer and the equation of statistical equilibrium. When a photon propagates with a distance \( (ds) \), the intensity \( (I_v) \) at a frequency of \( \nu \) varies as

\[
\frac{dI_v}{ds} = j_v - \alpha_v I_v,
\]

\( (40) \)

where \( j_v \) and \( \alpha_v \) are the local emission and absorption coefficients, respectively. These coefficients are related to the properties of molecules and dust particles.
Figure 7. Gas temperature (image) and CO abundance (contour), as a function of visual extinction (A_V) and the total hydrogen density (n), for a given FUV strength (presented inside boxes) with the Draine field. The black, gray, and white solid contours indicate the CO abundances of 10^{-6}, 10^{-5}, and 10^{-4}, respectively. The white dashed contour represents the gas temperature of 300 K. The two vertical and horizontal dotted lines represent the lines for A_V = 0.1 and 1, and log n = 6 and 7, respectively. (A color version of this figure is available in the online journal.)

For molecular radiation, each transition has the two coefficients as

\[ j_i^{(\text{gas})} = \frac{h v_i}{4\pi} n_u A_{ul} \phi_i(v) \]  

(41)

\[ \alpha_i^{(\text{gas})} = \frac{h v_i}{4\pi} (n_l B_{lu} - n_u B_{ul}) \phi_i(v), \]  

(42)

where \( A_{ul}, B_{ul}, \) and \( B_{lu} \) are the Einstein coefficients. \( n_l \) and \( n_u \) are lower and upper level populations, respectively. \( h v_i \) is the energy difference between the lower and upper levels. The line profile is assumed to be a Doppler profile:

\[ \phi_i(v) = \frac{1}{\sigma \sqrt{\pi}} \exp \left[ -\left( v - v_i - v \cdot \mathbf{n} \frac{v_i}{c} \right)^2 / \sigma^2 \right], \]  

(43)

where \( \sigma \) is the Doppler width and \( v_i \) is the center frequency of the transition, \( v \) is the local velocity field, and \( \mathbf{n} \) is the direction vector of the photon-propagation. Our code considers line overlap in complex molecules. The two coefficients for the molecules are

\[ j_i^{(\text{gas})} = \sum j_i^{(\text{gas})} \]  

(44)

\[ \alpha_i^{(\text{gas})} = \sum \alpha_i^{(\text{gas})}. \]  

(45)

For dust continuum radiation, the two coefficients are

\[ j_i^{(\text{dust})} = \alpha_i^{(\text{dust})} B_\nu(T_{\text{dust}}) \]  

(46)

\[ \alpha_i^{(\text{dust})} = k_\nu \rho_{\text{dust}}, \]  

(47)

where \( B_\nu \) is the Planck function for a given dust temperature. \( k_\nu \) and \( \rho_{\text{dust}} \) are the dust opacity and density, respectively.

When we calculate the local radiation field, we determine the level populations through the equation of statistical equilibrium:

\[ n_l \left[ \sum_{k<l} A_{lk} + \sum_{k \neq l} (B_{lk} \bar{J}_{lk} + C_{lk}) \right] = \sum_{k>l} n_k A_{lk} + \sum_{k \neq l} n_k (B_{kl} \bar{J}_{kl} + C_{kl}), \]  

(48)

where \( C_{kl} (C_{lk}) \) is the collision rate from level \( k \) to \( l \) and \( \bar{J}_{lk} \) is

\[ \bar{J}_{lk} = \int d\Omega \int d\nu I_\nu \phi_{lk}(v). \]  

(49)
RATRAN solves the line radiative transfer using an accelerated Monte Carlo method, which splits \( \bar{J}_{lk} \) into a local contribution and an external field,

\[
\bar{J}_{lk} = \bar{J}_{lk}^{\text{external}} + \bar{J}_{lk}^{\text{local}} \tag{50}
\]
or, in view of model photons,

\[
\bar{J}_{lk} = \left[ \sum_i I_{lk}^{\text{ext}} e^{-\tau_i} \phi_{hl}(v_i) + \sum_i S_{\nu i} (1 - e^{-\tau_i}) \phi_{hl}(v_i) \right] \left/ \sum_i \phi_{hl}(v_i) \right. \tag{51}
\]

\( I_{lk}^{\text{ext}} \) is the intensity entering into the local cell, \( \tau_i \) (the local optical depth), and \( S_{\nu i} \) (the local source function) are given as

\[
\tau_i = (\alpha_{\nu i} (\text{gas}) + \alpha_{\nu i} (\text{dust})) \cdot ds \tag{52}
\]

\[
S_{\nu i} = \frac{j_{\nu i} (\text{gas}) + j_{\nu i} (\text{dust})}{\alpha_{\nu i} (\text{gas}) + \alpha_{\nu i} (\text{dust})} \tag{53}
\]

RATRAN finds a local solution for a grid by solving the equation of the statistical equilibrium and the local radiation field for the given external radiation field, then finds a global solution for all grids. We have upgraded the local solution-finding method with “newt” subroutine (Press et al. 1992) in RIG, which can cope with line overlaps among multiple molecular and atomic species. We also update “SKY” in RATRAN to make a spectral image in the general coordinate for any given inclination.

3. BENCHMARKING

3.1. Non-LTE Line Radiative Transfer in the \((r, \delta)\) Coordinates

In order to confirm that the ray-tracing scheme in the \((r, \delta)\) coordinates is reliable, we compare RIG with the \((r, \delta)\) coordinate system with 1D RATRAN. For this test, we run the benchmark test of model 2b in van Zadelhoff et al. (2002). This is an analytical inside-out collapse model (Shu 1977) of B335 for an optically thick case with a constant abundance of HCO\(^+\) of \(1 \times 10^{-8}\). The benchmark test shows that the differences among participating models are 2% and 20% in \(J = 1\) and \(J = 4\), respectively (van Zadelhoff et al. 2002). For this test, we divide the envelope with the spherical symmetric density structure into three \(\delta\) regions: R1, R2, and R3, as shown in the left panel of Figure 3. The three regions should have the

\footnote{http://www.strw.leidenuniv.nl/astrochem/radtrans/}
The two codes used the same 100 grid cells from 30 AU to 30,000 AU. Figure 4 shows that the results by two codes are very consistent. $A_V$ on the top axis is derived from the relation between $A_V$ and the column density of hydrogen. The average visual extinction $\langle A_V \rangle$, which is derived by Equation (12), is higher than $A_V$ as the scattering is more forward-directed. However, for the pure forward scattering ($g = 1.0$), which has an analytic solution using the relation between $A_V$ and the column density of hydrogen, $\langle A_V \rangle$ is only 1% different from $A_V$ when the albedo is considered. Therefore, our FUV radiative transfer code is reliable.

### 3.3. Thermo-chemical Part of PDR

In order to test the reliability of our PDR code, we have run the four benchmark tests described in the PDR comparison study by R07: V1 ($n = 10^3$ cm$^{-3}$ and $\chi = 10$), V2 ($n = 10^5$ cm$^{-3}$ and $\chi = 10^5$), V3 ($n = 10^{5.5}$ cm$^{-3}$ and $\chi = 10$), and V4 ($n = 10^{5.5}$ cm$^{-3}$ and $\chi = 10^5$). These tests calculate the gas temperature and the chemistry self-consistently. A cloud with 1D slab geometry is assumed to be illuminated by an UV field in only one side. The same model parameters (Table 5 of R07), chemical species, and chemical reactions as those for the benchmark tests are used. As a result, we use the simple H$_2$ formation rate of $R_{H_2} = 3 \times 10^{-18} \sqrt{T_{\text{gas}} n n_H}$ instead of Equation (25) and the formula of Bakes & Tielens (1994) instead of Equations (28).
Figure 10. Rotational temperature $T_{\text{rot}}$ (contour) and emitting CO number in $J = 24$ $N(24)$ (image), as a function of visual extinction ($A_V$) and the total hydrogen density ($n$), for a given FUV strength in the Draine field. $N(24)$ is calculated with the LVG model, and $T_{\text{rot}}$ is fitted from $J = 14$ to $J = 24$ (see the text).

(A color version of this figure is available in the online journal.)

Figures 5 and 6 show the results of our PDR model (PDR_S) compared to those of other codes in R076: Cloudy (e.g., Abel et al. 2005), Costar (Kamp & van Zadelhoff 2001), htbkw (e.g., Tielens Hollenbach 1985), Kosma-tau (e.g., Röllig et al. 2006), leiden (e.g., Jansen et al. 1995), Meijerink (Meijerink & Spaans 2005), meudon (e.g., Le Petit et al. 2004), stenberg (e.g., Sternberg & Dalgarno 1989), and ucl-pdr (e.g., Bell et al. 2006). The overall agreement is very good, and the results of our PDR model fall within the scatter of the results produced by other codes. Therefore, our PDR model is reliable enough to be applied to more complicated models.

The only notable difference between our model and others in R07 is the gas temperature of the V2 model (see the right column in Figure 1). We use the updated collision rate coefficients of an O atom with atomic hydrogen (Abrahamsson et al. 2007), which are larger than previous calculations by Launay & Roueff (1977) (used in other models) by a factor of 2–3 at a temperature near 1000 K. Therefore, our V2 model has higher [O i] cooling rates resulting in lower gas temperatures in the lower $A_V$.

4. 1D PDR MODEL FOR WARM CO

Before running a 2D model, we have made simple tests to check the PDR contribution to the FIR mid-$J$ ($14 \leq J \leq 24$) CO transitions with the 1D model. We have run the plane-parallel 1D model, similar to the benchmark tests, with our full chemistry and gas energetics. Though an approximated formula for the dust temperature in BB1.5 and BB1.0 is different from that in the Draine field (Spaans et al. 1994), we use the same equation in Section 3. The explored parameter space is $2.0 \leq \log n \leq 9.0$ and $0.0 \leq \log G_0 \leq 6.0$ with a step of 0.5.

Figures 7–9 show the gas temperature and CO abundance X(CO) in each physical point for the models with the Draine field, BB1.5, and BB1.0, respectively. The gas temperature is determined by the thermal balance between heating and cooling described in Section 2.4. As seen in Figures 7–9, the gas temperature is not a simple function of density. For log $G_0 > 4.0$, the gas temperature has a dip at a range of density; for example, for log $G_0 = 6$, the temperature dip appears around

http://www.astro.uni-koeln.de/site/pdr-comparison/
This nonlinearity of temperature occurs because of the different dependence of density in heating and cooling. In the physical conditions of test models, the dominant heating and cooling mechanisms are photoelectric heating by PAHs and small grains and the [O\textsc{I}] 63 \mu m emission line, respectively. The photoelectric heating rate is proportional to \( n^p \) and \( 1 < p < 2 \). However, the cooling rate by the [O\textsc{I}] line is proportional to \( n^2 \) and \( n \) if the density is smaller and greater than the critical density (\( \sim 10^5 \text{ cm}^{-3} \)) of the [O\textsc{I}] line, respectively (see Section 3.1 of Kaufman et al. (1999) for detailed explanations). As a result, these two combinations of different power indexes with density make the temperature dip, which appears at different densities depending on the UV spectral type and the UV strength.

As the FUV strength increases in the dense region (\( \log n \geq 6 \)), the gas temperature also grows and more CO molecules are photodissociated near the surface. Interestingly, when log \( G_0 \geq 4 \), CO molecules survive even in the warm region with log \( X(\text{CO}) \geq -5 \), which could emit the FIR mid-\( J \) CO lines observed by \textit{Herschel}/PACS. A high gas temperature enhances the CO formation rate to survive in this condition (see below). The models with BB1.5 and BB1.0 have slightly lower gas temperatures and higher CO abundances near the surface than the model with the Draine field.

Because it is a simple 1D plane parallel model, we calculate the number of emitting CO molecules at the FIR mid-\( J \) transitions with large velocity gradient code RADEX (van der Tak et al. 2007). We assume that the total hydrogen column density \( N(\text{H}) \) per visual extinction \( A_V \) is \( 1.87 \times 10^{21} \text{ cm}^{-2} \), the column density of CO \( N(\text{CO}) \) at each \( A_V \) position is the product of \( N(\text{H}) \) and the local CO abundance, and the line width is 1.0 km s\(^{-1} \). Then the normalized level population in \( J \) (\( n(J) \); \( \sum n(J) = 1 \)) is calculated with RADEX.

The number of CO emitting in the \( J \) level, \( N(J) \), is defined as

\[
N(J) \simeq n(J) \times N(\text{CO}) \times \left[ \frac{10^4}{G_0} \times (100 \text{ AU})^2 \right].
\]  

The brackets enclose the area correction factor if the UV luminosity of the central source (\( L_{\text{UV}} \)) is 0.1 \( L_\odot \). At given \( L_{\text{UV}} \), the unattenuated FUV strength \( G_0 \) is approximated as

\[
G_0 \simeq 10^4 \frac{L_{\text{UV}}}{0.1 L_\odot} \left( \frac{r}{100 \text{ AU}} \right)^{-2},
\]  

where \( r \) is the distance from the central source. Therefore, the area exposed to the unattenuated FUV strength \( G_0 \) is proportional to \( r^2 \) and thus to \( 1/G_0 \).

Figures 10–12 show \( N(24) \) and the rotational temperature \( T_{\text{rot}} \) fitted from \( J = 14 \) to \( J = 24 \) for the models with the Draine field, BB1.5, and BB1.0, respectively. The CO \( J = 24–23 \) transition traces the warm component of \( T_{\text{rot}} \geq 300 \text{K} \) and is
emitted from near the surface ($0.1 \leq A_V \leq 1$) of dense region ($6 \leq \log n \leq 8$) with high FUV strength ($\log G_0 \geq 3.5$). These regions are in a few hundred AU from the protostar. When the FUV strength increases for the same density, for example, $\log n = 7$, most fluxes of the mid-$J$ CO transitions are emitted with similar $T_{\text{rot}}$ but from deeper $A_V$. This can explain why $T_{\text{rot}}$ has a universal value, independent of bolometric luminosity and density of embedded protostars.

The CO $J = 14–13$ line is emitted from the deeper region than the CO $J = 24–23$ line (see Figures 13–15). As this line traces the cool component ($T_{\text{rot}} \simeq 100$ K) as well as the warm one, we should run the 2D PDR models to check whether the PDR model can produce the FIR mid-$J$ CO lines observed by Herschel/PACS. Models with BB1.5 and BB1.0 have higher $N(24)$ and $N(14)$, but lower $T_{\text{rot}}$ than the model with the Draine field.

5. UV HEATED OUTFLOW CAVITY WALLS FOR HH46

We have applied our PDR model to the UV-heated outflow cavity walls for HH46 following the models of Visser et al. (2012) and Bruderer et al. (2009a). The CO ladders observed by Herschel/PACS in HH46 show that two temperature (warm and hot) gas components are indicative in the rotation diagram, and the warm component has $T_{\text{rot}} \simeq 300$ K, which is possibly produced by UV photons (Visser et al. 2012).

5.1. Model

A density distribution of the envelope is assumed to be a power law of the spherically symmetric 1D model, except for the outflow cavity. We adopt the density structure of envelope from Visser et al. (2012),

$$n = 2.2 \times 10^9 \left(\frac{r}{34.6 \text{ AU}}\right)^{-2.0} \text{ cm}^{-3}. \quad (56)$$

The outflow cavity is carved out with the opening angle of 60° by Equation (2). We assume that the density inside the outflow cavity is $1.2 \times 10^4 \text{ cm}^{-3}$ (Neufeld et al. 2009; Visser et al. 2012). The dust temperature is calculated with RADMC-3D adopting the same dust opacity used in Section 2.2. We choose the stellar temperature of 5000 K, which does not significantly affect the dust temperature in the envelope (Visser et al. 2012). The bolometric luminosity of 27.9 $L_\odot$ is adopted as the luminosity of the internal source (Karska et al. 2013). Figure 16 (upper panels) shows the dust temperature distribution calculated by RADMC-3D in the 2D spherical coordinate system ($r$, $\theta$) with 360 (in $r$) $\times$ 300 (in $\theta$) grid cells. For the PDR model, we use the ($r$, $\delta$) coordinates, where $r$ is the radial distance from the central
The dust temperature \( T_{\text{dust}}(r, \theta) \) from RADMC-3D is therefore converted to \( T_{\text{dust}} \) in the \((r, \delta)\) coordinates by

\[
T_{\text{dust}} = \frac{\int_{r_{\text{min}}}^{r_{\text{max}}} r^2 \int_{\cos\theta(r, \delta_{\text{max}})}^{\cos\theta(r, \delta_{\text{min}})} T_{\text{dust}}(r, \theta) n(r, \theta) d(\cos\theta) \, dr \int_{r_{\text{min}}}^{r_{\text{max}}} r^2 \int_{\cos\theta(r, \delta_{\text{max}})}^{\cos\theta(r, \delta_{\text{min}})} n(r, \theta) d(\cos\theta) \, dr }{\int_{r_{\text{min}}}^{r_{\text{max}}} r^2 \int_{\cos\theta(r, \delta_{\text{max}})}^{\cos\theta(r, \delta_{\text{min}})} n(r, \theta) d(\cos\theta) \, dr }, \tag{57}
\]

where \( n(r, \theta) \) is the total hydrogen number density and \( \cos\theta(r, \delta) \) is the \( \cos\theta \) for the given \((r, \delta)\) grid point. The \( r \) and \( \delta \) grids are plotted as vertical and curved lines, respectively, in Figure 16. The dust temperature distribution is well described by the \((r, \delta)\) grids.

The \( \delta \) coordinate is an adequate coordinate system to describe the outflow structure and resolve the very narrow regions near the outflow wall surface where the warm CO gas exists, as shown in Figure 16. In addition, both PDR and non-LTE line radiative transfer calculations should be able to deal with scales ranging from \( \sim 10 \) AU to \( \sim 10^3 \) AU. Properties of the PDRs are characterized by three parameters: a density, an unattenuated (or incident) FUV strength, and a depth \( (A_V) \) or a column density of hydrogen. As the density profile of the envelope is assumed to be a power law of radial distance and the incident FUV strength follows an inverse square law of the radial distance, \( r \), which is equidistant on a logarithmic scale as shown as vertical lines in Figure 16, has been chosen.

\( A_V \) is described by a column density in the 1D models. As photons from the central protostar propagate radially (horizontally in Figure 16), radial points are first calculated to have an equivalent interval in \( \log A_V \) from the outflow wall surface along the horizontal direction at \( r = 1000 \) AU, as shown with the white arrow in Figure 16, and then Equation (12) is used to trace \( \delta \) grids for the found radial points and \( \cos\theta \) of 0.28. At \( r = 1000 \) AU, the \( \delta \) point closest to the outflow surface has \( A_V = 0.1 \), and the deepest \( \delta \) point has \( A_V = 10 \) in Figure 16.

The \( \delta \) coordinate presents well the very narrow layer near the outflow surface for \( A_V \lesssim 1 \), where the mid-\( J \) CO emission is radiated as seen in the 1D models. In addition, the FUV strength near the surface drops by an order of magnitude (see the bottom right panel of Figure 16), requiring a high resolution. Therefore, we calculate the FUV radiative transfer in the \((r, \delta)\) coordinate system instead of using the result of RADMC-3D because 30 \((\log r) \times 10\) (in \( \delta \)) grid cells can provide a higher spatial resolution (for the FUV strength near the surface) than 360 \((\log r) \times 300\) (in \( \cos\theta \)) in the spherical coordinates. However, the dust temperature is calculated by RADMC-3D because the dust temperature varies only within 10 K near the surface, and a higher resolution does not affect results.

As the mid-\( J \) CO emission is the major concern for this model, half of the \( \delta \) grids are put near the surface to provide a enough spatial resolution in the UV heated cavity walls. A larger number
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Figure 14. Same as Figure 13 except for BB1.5.
(A color version of this figure is available in the online journal.)

of grids (90 in \( \log r \) and 30 in \( \delta \)) show a similar result to the 300 grid model. We note that our PDR model with 300 grids cannot describe sharp transitions of H-H\(_2\) and C+-C-CO, which do not affect our result.

We assume that the central protostar is the only FUV source. The initial FUV radiation field stored in each photon package is given by

\[
I_0 = \frac{L_{\text{uv}}}{N_{\text{phot}}},
\]

where \( L_{\text{uv}} \) is the FUV luminosity of the central protostar and \( N_{\text{phot}} \) is the number of photons. The photon packages initially propagate the system in the radial direction, and they are traced until they escape from the outer boundaries of both the outflow cavity and the envelope.

As presented in Figure 17, we have run a comparison model as well as our self-consistent models for the different UV radiation fields (BB1.0, BB1.5, and the Draine field). For the comparison model (Figure 17), we have followed the method of Visser et al. (2012) (hereafter V12 model). In this method, the gas temperature has been calculated from an approximated formula, \( T(G_0, A_V) = T_S \exp(-0.6 A_V) \), where the surface temperature \( T_S \) was adopted from Kaufman et al. (1999), and the chemistry has been calculated with BB1.0.

The FUV observation toward classical T Tauri stars shows that the UV luminosity integrated from 1250 Å to 1750 Å (\( L_{\text{Int}}^{\text{uv}} \)) is related with the accretion luminosity (\( L_{\text{acc}} \)) as

\[
\log L_{\text{Int}}^{\text{uv}} = 0.836 \times \log L_{\text{acc}} - 1.67
\]

with an accuracy of 0.38 dex (Yang et al. 2012). As the FUV luminosity integrated from 912 Å to 2050 Å is about two times \( L_{\text{Int}}^{\text{uv}} \) for TW Hya and AU Mic (Yang et al. 2012) and the accretion luminosity dominates the bolometric luminosity during the class 0 and I, we adopt a reference UV luminosity of \( L_{\text{YUV}}^{\text{uv}} = 0.7 L_\odot (0.02 L_\odot) \).

Level population and spectral images are calculated with RIG, which can solve the problem with the same coordinates used in the PDR model. The CO molecular data file (Neufeld 2012) is adopted from the Leiden Atomic and Molecular Database\(^7\) (Schöier et al. 2005). Spectral images at the known inclination of HH46 (\( i = 53^\circ \)) are synthesized with a spatial resolution of 0′′05 (23 AU at distance of HH46) and a spectral resolution of 0.1 km s\(^{-1}\). As most emission is from near the center of the image, the intensity over the PACS 5 × 5 spaxels (50′′×50′′) is summed.

5.2. Results

In this section, we find the best fit UV luminosity inferred from our models that fit the Herschel/PACS observations.

\(^7\) http://home.strw.leidenuniv.nl/~moldata/datafiles/co@neufeld.dat
The rotational diagrams from CO ladders detectable with Herschel/PACS are plotted in Figure 17. The number of CO emitting in the J level is calculated as follows: Green et al. (2013):

$$N_{\text{OBS}}(J) = \frac{4\pi D^2 F_J}{h \nu_J A},$$  \hspace{1cm} (59)

where $F_J$ and $\nu_J$ denote the line flux and the frequency of the CO rotational transition from $J$ to $J-1$, $D$ is the distance to the source, $A$ is the Einstein coefficient, and $h$ is Planck’s constant.

Figure 18 shows the 2D structure of the dust attenuated FUV strength $G_{\text{dust}}$ (top left), average visual extinction $\langle A_V \rangle$ (top right), gas temperature $T_{\text{gas}}$ (bottom left), and dust temperature $T_{\text{dust}}$ (bottom right) for the HH46 model. The color scales of $G_{\text{dust}}$ and $T_{\text{dust}}$ are the same as those in Figure 16, and $G_{\text{dust}}$ calculated by RADMC-3D and our code are similar. $\langle A_V \rangle$ along the equatorial plane decreases outward because $G_{\text{dust}}$ is almost constant in this scale while unattenuated FUV strength $G_0$, which can be approximated by the dust attenuated FUV strength in the outflow cavity, drops because of the inverse square law of distance (see Equation (12)). Scattered UV photons that come through the surface in higher $z$ pass lower column densities compared to photons passing through near the equatorial plane. As a result, $G_{\text{dust}}$ is nearly constant in large scale.

Horizontal distributions of physical and chemical properties for given $z$-heights are plotted in Figures 19–21. The given $z$-heights are marked with horizontal color lines and the same color text in top left panel of Figure 19. Other panels show the physical values along the horizontal lines from the surface of the outflow cavity wall for given $z$-heights. Filled circles and open squares plotted over each line indicate grid cells where most emission from $J = 24$–$23$ and $J = 14$–$13$ is radiated, respectively. The filled squares in the plots present the grid cells where both lines of $J = 24$–$23$ and $J = 14$–$13$ contribute to the total emission similarly. $J = 14$ and 24 are the lowest and highest upper levels for the representative transitions in the warm component of CO gas. If a grid has a volume of $V$, the CO abundance of $X(\text{CO})$, and the population in the $J$ level $n(J)$, the normalized number of CO in the $J$ level $N^n(J)$ is defined as follows:

$$N^n(J) = \frac{n(J) X(\text{CO}) V}{N_{\text{OBS}}(J)},$$  \hspace{1cm} (60)

where $N_{\text{OBS}}(J)$ is the observed value described in Equation (59). We note that the distribution of the density (top right of Figure 19), the FUV strength (bottom left of Figure 19), and the dust temperature (bottom right of Figure 19) are the same for all models of different UV spectral types. However, the absolute values of $G_{\text{dust}}$ vary with the UV luminosity that fits the observations. In Figure 19, $G_{\text{dust}}$ for the best-fit model of BB1.5 are plotted. Figures 20 and 21 show the horizontal distribution...
Figure 16. $r$ and $\cos \theta$ diagrams for the dust temperature $T_{\text{dust}}$ and the attenuated FUV strength $G_{\text{dust}}$ calculated with RADMC. The $r$ and $\delta$ grids are plotted as vertical and curved lines, respectively. The right columns zoom in on the sub-region near the surface of the inner envelope. The $\delta$ grids describe well the distributions of dust temperature and the attenuated FUV strength in the deep envelope (left) as well as narrow outflow cavity wall surfaces (right) for the envelope model with outflow cavity. A column density is measured along the horizontal white arrow for setting the $\delta$ grids (see Section 5.1).

(A color version of this figure is available in the online journal.)

Figure 17. Rotational diagram of models for each UV radiation field. The blue line indicates the model calculated with the same method as Visser et al. (2012). The cyan, green, and orange lines indicate the model with BB1.0, BB1.5, and Draine field, respectively (see the text). Herschel/PACS observation data are plotted as red diamonds. Their rotational temperatures are fitted up to $E_{\text{up}} \lesssim 1800$ K, and the best fit UV luminosities in units of $L_{\text{UV}}^1(0.7 \ L_\odot)$ and rotational temperatures are presented inside the box.

(A color version of this figure is available in the online journal.)

of gas temperature ($T_{\text{gas}}$) and CO abundance ($X(\text{CO})$) for the models of V12, B1.0, B1.5, and the Draine field.

In the best-fit PDR models, the majority of mid-$J$ CO emission is radiated from the surface ($\Delta R \lesssim 10$ AU or $0.1 \lesssim A_V \lesssim 1$) of the inner dense UV heated cavity walls with $6 \lesssim \log n(\text{cm}^{-3}) \lesssim 8$, $X(\text{CO}) > 10^{-5}$, and $T_{\text{gas}} > 100$ K. The CO $J = 24-23$ transition traces mostly the warm gas ($T_{\text{gas}} \gtrsim 300$ K), while the CO $J = 14-13$ transition arises from both the warm and cool ($T_{\text{gas}} \simeq 100$ K) gas. Therefore, the contribution of the cool gas to the flux of CO $J = 14-13$ determines the synthesized rotational temperature.

Our V12 model results in a rotational temperature and FIR mid-$J$ fluxes similar to Visser et al. (2012) with 30% enhanced UV luminosity. Though the FUV radiative transfer and chemistry (especially H$_2$ formation rate) of our model are slightly different from those of Visser et al. (2012), synthesized CO fluxes are similar in two models. Our self-consistent PDR model with BB1.0 also shows a rotational temperature similar to that of the V12 model, but UV luminosity seven times larger is required to match the observation. The fitted UV luminosity for BB1.0 (1.0 $L_{\text{UV}}^1$) is same as the value derived from the observational relation of the classical T-Tauri stars (see above). This result indicates that the approximation of gas temperature and the inconsistency of UV field in the gas energetics and chemistry adopted by Visser et al. (2012) might underestimate the UV luminosity of the source.
Figure 18. Physical structure of HH46 with BB1.5: dust attenuated FUV strength (top left), average visual extinction \(\langle A_V \rangle\) (top right), gas temperature (bottom left), and the dust temperature structure (bottom right). The gas temperature is calculated with our PDR model (Section 2), but the dust temperature is calculated with RADMC-3D (Section 5.1).

(A color version of this figure is available in the online journal.)

Figure 19. Density (top right), FUV strength (bottom left), and dust temperature (bottom right) distributions along given horizontal cuts in the envelope of HH46. Each color line indicates the physical values for a given z-height, which is represented with the same color in the top left panel. \(\Delta R\) is the horizontal distance from the outflow cavity wall surface. The filled circles, open squares, and filled squares on top of the lines indicate the grid cells where emissions of \(J = 24\)–23, 14–13, and both lines are radiated, respectively.

(A color version of this figure is available in the online journal.)
Figure 20. Gas temperature (left column) and CO abundance (right column) of best-fit models. The top and bottom panels indicate the model for V12 and BB1.0, respectively. The colored lines are the same as presented in Figure 19.

(A color version of this figure is available in the online journal.)

Figure 21. Same as Figure 20 except for the best fit models of BB1.5 (top) and the Draine field (bottom).

(A color version of this figure is available in the online journal.)
Unlike the V12 model, our self-consistent PDR models with BB1.5 and the Draine field can reproduce the observed fluxes in the mid-\(J\) CO transitions (\(E_{\text{up}} \leq 1800\) K) without additional heating by a shock, which was adopted by Visser et al. (2012), if the UV luminosity is 3.5 \(L_{\text{UV}}^\star\) (2.4 \(L_\odot\)). Of course, the line fluxes for \(J\) levels with \(E_{\text{up}} > 1800\) K cannot be reproduced by the PDR, which is indicative of shock contribution in the high-\(J\) CO lines. However, the important point here is that a self-consistent calculation of PDR could be important to constrain the UV radiation field associated with the accretion process in an embedded protostar.

Our PDR model with BB1.0 has a lower gas temperature than that of V12 model for the same UV luminosity. A higher UV luminosity increases the gas temperature, but it also reduces the CO abundance near the surface. Hence, the model with BB1.0 needs UV luminosity about seven times larger to produce similar fluxes to V12 model.

BB1.5 has a photodissociation rate of CO two times lower than the Draine field. The best fit model with BB1.5 has a slightly lower gas temperature (by about 10%) but a slightly higher CO abundance than the best fit model with the Draine field (see Figure 21), which results in similar CO fluxes.

Generally, in a dense PDR (log \(n \geq 6\)), a higher \(G_0/n\) results in a higher gas temperature and a lower CO abundance near the surface. Because the density profile and FUV strength both follow the inverse square law of the radius, \(G_0/n\) is almost constant near the surface, and \(\langle A_V\rangle\) decreases as \(z\) is lowered. Therefore, the CO abundance near the surface decreases toward lower \(z\). However, along the surface of the outflow cavity walls, the CO abundance sharply increases from \(n \sim 10^6\) cm\(^{-3}\) (\(z = 500\) AU; the green line in Figure 21) inward to reach \(X(\text{CO}) \gtrsim 10^{-5}\), where the FIR mid-\(J\) CO emission is radiated.

Distributions of CO abundance in the domain of \(A_V\) and \(T_{\text{gas}}\) for a given FUV strength and gas density (log \(n = 7\) cm\(^{-3}\)) are
plotted in Figure 22. For log $G_0/n \sim -3$ (G4.0; middle row), near the surface (low $A_V$), there is the abundance jump around the gas temperature of a few hundred Kelvin. For example, the model of BB1.5 with the FUV strength of $10^4$ ISRF (G4.0 BB1.5) has an abundance below $10^{-7}$ at $T_{\text{gas}} < 300$ K, but has the abundance above $10^{-5}$ in the gas temperature higher than 500 K. In this temperature region, CO forms fast through following reactions (Burton et al. 1990):

$$\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H} \quad (61)$$

$$\text{OH} + \text{C}^+ \rightarrow \text{CO}^+ + \text{H} \quad (62)$$

$$\text{CO}^+ + \text{H}_2 \rightarrow \text{HCO}^+ + \text{H} \quad (63)$$

$$\text{HCO}^+ + e^- \rightarrow \text{CO} + \text{H}_2 \quad (64)$$

and near the surface (or higher $G_0/n$), instead of Equations (63) and (64), through the reaction

$$\text{CO}^+ + \text{H} \rightarrow \text{CO} + \text{H}^+ \quad (65)$$

This jump in the CO abundance depends on $G_0/n$ and the radiation field. In a higher $G_0/n$ and the UV radiation field of a higher effective temperature blackbody, the CO abundance jump occurs at a deeper region with a higher gas temperature due to the more efficient photodissociation at the same $A_V$. For our best fit model with BB1.5, most fluxes of the mid-J CO lines are emitted from the condition of log $G_0/n \sim -3$ and $0.1 \leq A_V \leq 1.0$, where the CO abundances increase from $\sim 300$ K.

6. SUMMARY

We have developed a self-consistent PDR model with an optimized coordinate system to the embedded protostars with outflow cavities, which reduces a number of grid and a calculation time with no loss of information. The benchmark test shows that our model agrees with other models in R07.

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