Circumnuclear Multi-phase Gas in the Circinus Galaxy. I. Non-LTE Calculations of CO Lines

Keiichi Wada1,2,3, Ryosuke Fukushige1, Takuma Izumi4,5, and Kohji Tomisaka4

1 Kagoshima University, Graduate School of Science and Engineering, Kagoshima 890-0065, Japan; wada@astrophysics.jp
2 Ehime University, Research Center for Space and Cosmic Evolution, Matsuyama 790-8577, Japan
3 Hokkaido University, Faculty of Science, Sapporo 060-0810, Japan
4 National Astronomical Observatory of Japan, Mitaka 181-8588, Japan
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Abstract

In this study, we investigate the line emissions from cold molecular gas based on our previous “radiation-driven fountain model,” which reliably explains the spectral energy distribution of the nearest type 2 Seyfert galaxy, the Circinus galaxy. Using a snapshot of the best-fit radiation-hydrodynamic model for the central r ≤ 16 pc, in which non-equilibrium X-ray-dominated region chemistry is solved, we conduct post-processed non-local thermodynamic equilibrium radiation transfer simulations for the CO lines. We obtain a spectral line energy distribution with a peak around J ≈ 6, and its distribution suggests that the lines are not thermalized. However, for a given line of sight, the optical depth distribution is highly non-uniform between τ0 ≤ 1 and τ0 ≫ 1. The CO-to-H2 conversion factor (XCO), which can be directly obtained from the results and is not a constant, depends strongly on the integrated intensity and differs from the fiducial value for local objects. XCO exhibits a large dispersion of more than one order of magnitude, reflecting the non-uniform internal structure of a “torus.” In addition, we found that the physical conditions differ between grid cells on a scale of a few parsecs along the observed lines of sight; therefore, a specific observed line ratio does not necessarily represent a single physical state of the interstellar medium.

Key words: galaxies: active – galaxies: ISM – galaxies: nuclei – radiative transfer – radio lines: ISM

1. Introduction

In the standard picture of active galactic nuclei (AGNs), the nucleus is hypothetically surrounded by an optically and geometrically thick “dusty torus.” Except for a few nearby AGNs, such as NGC 1068, NGC 1097, and the Circinus galaxy (e.g., Jaffe et al. 2004; Tristram et al. 2014; Gallimore et al. 2016; García-Burillo et al. 2016; Imanishi et al. 2016; Izumi et al. 2017), dust and molecular emissions have not yet been spatially resolved; therefore, the real geometrical and internal structures of the tori are still unclear. The origin and physical mechanism of the obscuring material around the nucleus have been widely discussed by many authors (e.g., Krolik & Begelman 1988; Pier & Krolik 1993; Ohsuga & Umemura 2001; Lawrence & Elvis 2010; Hopkins et al. 2012). Recent time-dependent radiation-(magneto)hydrodynamic simulations commonly suggested that a static, donut-like torus is not reproduced, because the interstellar medium (ISM) is very dynamic on the scale of sub-parsec to tens of parsecs (Dorodnitsyn et al. 2012, 2016; Wada 2012; Chan & Krolik 2016, 2017; Namekata & Umemura 2016; Wada et al. 2016; Dorodnitsyn & Kallman 2017), although there are non-negligible differences in the results among the simulations.

Wada (2012) proposed that the obscuring structures around AGNs, in which outflowing and inflowing gases are driven by radiation from the accretion disk, form a geometrically thick disk on the scale of a few parsecs to tens of parsecs. The quasi-steady circulation of gas, i.e., the “radiation-driven fountain,” may obscure the central source; therefore, the differences in the spectral energy distributions (SEDs) of typical type 1 and 2 Seyfert galaxies are reliably explained (Schartmann et al. 2014). Wada (2015) showed that the observed properties of obscured AGNs change as a function of their luminosity because of fountain flows, and the results were compared with recent X-ray and infrared observations (see also Ramos Almeida & Ricci 2017).

Wada et al. (2016; hereafter W16) applied this radiation-driven fountain model to the Circinus galaxy, which is the nearest (D = 4 Mpc) type-2 Seyfert galaxy. We studied, for the first time, the non-equilibrium chemistry for the X-ray-dominated region (XDR) with supernova feedback in the central r ≤ 16 pc. A double hollow cone structure occupied by an inhomogeneous, diffuse ionized gas is formed, and it is surrounded by geometrically thick (h/r ≲ 1) atomic/molecular gas. Dense molecular gases (e.g., H2 and CO with nH2 ≥ 1013 cm−3) are mostly concentrated around the equatorial plane, and atomic gas (e.g., H and C) extends with a larger scale height. The energy feedback from supernovae enhances its scale height. In W16, by applying post-processed three-dimensional (3D) radiation transfer calculations, we found “polar” emission in the mid-infrared band (12 μm), which is associated with bipolar outflows, as suggested in recent interferometric observations of nearby AGNs (Hönig et al. 2013; Tristram et al. 2014, see also Stalevski et al. 2017 for a theoretical model). In addition, we confirmed that the viewing angle θ, for the nucleus should be larger than 75° (i.e., close to edge-on) in order to explain the observed SED and 10 μm absorption feature of the Circinus galaxy (Prieto et al. 2010).

In this study, we focus on the structures of the cold molecular gas located in the outskirts of the infrared bright region in the best-fit model for the Circinus galaxy. In order to

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5 NAOJ Fellow.

6 The photon dominated region (PDR) chemistry and shock chemistry are not considered in the present model.
compare with future high-resolution observations of the molecular gas, we performed 3D non-local thermodynamic equilibrium (non-LTE) radiative transfer calculations for the $^{12}\text{CO}$ lines. Spatial distributions of the multi-$J$ line intensity, line ratios, spectral line energy distribution (SLED), and CO-to-H$_2$ conversion factor are discussed in the central 10 parsecs with a sub-parsec resolution. The results can be a theoretical reference to understand observations of the Atacama Large Millimeter/submillimeter Array (ALMA), whose spatial resolution can now reach a few parsecs in nearby AGNs. Detailed comparisons between the models and our Cycle-4 observations by ALMA will be discussed in a subsequent paper (T. Izumi et al. 2018, in preparation). The results of other molecules (e.g., HCN) and atomic gases (e.g., neutral carbon and hydrogen) will be discussed elsewhere.

2. Numerical Methods and Models

2.1. Input Model: Radiation-driven Fountain

We use a snapshot of our radiation-driven fountain model, which reliably explains the features of the SED of the Circinus galaxy (see details in W16). The results suggest that the viewing angle for the gas disk should be 75° or higher. We use our 3D Eulerian hydrodynamic code (Wada 2012, 2015), with a uniform grid that accounts for radiative feedback processes from the central source using a ray-tracing method. We include the non-equilibrium XDR chemistry (Maloney et al. 1996; Meijerink & Spaans 2005) for 256$^3$ zones (resolution of 0.125 pc). Self-gravity of the gas is ignored, because it is not essential for interpreting the gas dynamics in the radiation-driven fountain (see also Namekata & Umemura 2016). Supernova feedback is implemented in addition. Cooling functions for 20 K $\lesssim T_{\text{gas}} \lesssim 10^8$ K (Meijerink & Spaans 2005; Wada et al. 2009) and solar metallicity are assumed. At every time step, the gas density, $T_{\text{gas}}$ and $T_{\text{dust}}$, and ionization parameters in the 256$^3$ grid cells are passed to the chemistry module.

The central point mass is assumed to be $2 \times 10^6 M_\odot$, which is comparable to the value estimated from the maser observations (Greenhill et al. 2003), $1.7 \pm 0.3 \times 10^6 M_\odot$ in Circinus. The total gas mass is $2 \times 10^6 M_\odot$. The Eddington
ratio of 0.2 and the bolometric luminosity of $L_{\text{bol}} = 5 \times 10^{43}$ erg s$^{-1}$ are fixed during the calculation.

Here, we assume three independent radiation fields: (1) non-spherical ultraviolet (UV) radiation emitted from a thin accretion disk; (2) spherically symmetric X-ray radiation emitted from the corona of the accretion disk (Netzer 1987; Xu 2015); and (3) uniform far-UV (FUV) radiation arising from the star-forming regions that exist in the circumnuclear disk. All three components are assumed to be time-independent. The first component plays an important role in understanding the radiation pressure effects in the dust, whereas the second contributes primarily toward the heating of the gas and non-equilibrium XDR chemistry. The SED of the AGN and the dust absorption cross-section are taken from Laor & Draine (1993). The UV flux is assumed to be angle-dependent, i.e., $F_{\text{UV}}(\theta) \propto \cos \theta (1 + 2 \cos \theta)$ (Netzer 1987), where $\theta$ denotes the angle from the rotational axis ($z$-axis), which is calculated for all grid cells using 256$^3$ rays. The UV and X-ray fluxes are calculated from the bolometric luminosity (Marconi et al. 2004). The total X-ray luminosity (2–10 keV) is $L_X = 2.8 \times 10^{42}$ erg s$^{-1}$. The temperature of the interstellar dust $T_{\text{dust}}$ at a given position that is irradiated by the central UV radiation is calculated by assuming that thermal equilibrium has been attained (e.g., Nenkova et al. 2008); therefore, $T_{\text{dust}}$ is not necessarily equivalent to $T_{\text{gas}}$.

For simplicity, the third component of the radiation field, i.e., FUV, is assumed to be uniform. Instead of solving the radiation transfer for FUV in the inhomogeneous media with multi-radiation source—which is beyond our numerical treatment—we change its strength from $G_0 = 1000$ to $G_0 = 100$, where $G_0$ is the incident FUV field normalized to the local interstellar value ($1.6 \times 10^{-3}$ erg cm$^{-2}$ s$^{-1}$) and check whether it affects the results (see Section 4.2).

The 3D hydrodynamic grid data (i.e., density, temperature, abundances, and three components of velocity) of the 256$^3$ grid cells are averaged to produce 128$^3$ grid cells (i.e., the spatial resolution is 0.25 pc) in order to reduce the computational cost. This is passed to the 3D non-LTE line transfer code, as described in the next section, to derive the line intensities.

### 2.2. Non-LTE Line Transfer

The numerical code of the 3D line transfer calculations is the same as that used by Wada & Tomisaka (2005) and Yamada et al. (2007), which is based on the Monte–Carlo and long-characteristic transfer code (Hogerheijde & van der Tak 2000). The statistical equilibrium rate equations and the transfer equations are iteratively solved using photon packages (sampling rays) propagating into each grid cell. We solve the rate equations for the energy levels of $^{12}$CO from $J = 0$ to 15. Once the radiation field and optical depth are determined for all...
grid cells, we “observe” it from arbitrary directions, and 3D
data cubes (i.e., positions and line-of-sight velocity) are
obtained for selected transitions.
There are 1000 sampling rays for each grid cell. The level
populations are converged with an error of $10^{-6}$ for $J = 1$
and $10^{-3}$ for $J = 4$ after 10 iterations. The micro-turbulence, i.e., a
hypothetical turbulent motion inside one grid cell, is a free
parameter, which determines the shape of the line profile
function and varies from $v_{\text{turb}} = 1$ to $20 \text{ km s}^{-1}$. As a fiducial
value, we assume $v_{\text{turb}} = 10 \text{ km s}^{-1}$, and the effect of changing
$v_{\text{turb}}$ is discussed in Section 4. In contrast to previous papers
(Wada & Tomisaka 2005; Yamada et al. 2007), here we use the
non-uniform abundance distribution for $^{12}$CO, which is
obtained in the original radiation-hydrodynamic simulations
with XDR chemistry (W16). Note that $v_{\text{turb}}$ is different from the
typical velocity dispersion on the scale of several parsecs. In
fact, the average velocity dispersion of the gas in the input
model on a few parsecs is approximately $30 \text{ km s}^{-1}$, which is
consistent with the scale height of the cold ($< 100 \text{ K}$) molecular
gas seen in Figure 1. In the turbulent gas disk, the velocity
dispersion is increasingly larger with scale as might be expected from the power-law energy spectrum (e.g., Wada et al. 2002). Therefore, we expect that the velocity dispersion inside a grid cell should be smaller than the large-scale velocity dispersion. The “large-scale” bulk motion between grid cells in the disk is self-consistently considered in the non-LTE line transfer calculations.

Figure 1(a) presents spatial distributions of the $^{12}$CO abundance with respect to molecular hydrogen in the input model assuming $G_0 = 10^3$. As shown in Figure 1(b), the $^{12}$CO abundance is $x_{^{12}\text{CO}} = 10^{-5} - 10^{-4}$ for most grid cells, but there is large scatter for a given column density of the inhomogeneous disk. Hereafter, “CO” represents $^{12}$CO.

3. Results

3.1. Intensity Distribution

Figures 2 and 3 show the integrated intensity maps of CO
($1-0$) and the line ratio distributions ($J = 2-1/1-0, 3-2/1-0,$
and $4-3/1-0$) in $\text{K km s}^{-1}$ for the viewing angles $\theta_v = 0^\circ$
(i.e., face-on) and $75^\circ$, respectively. The intensity distributions
are morphologically similar between the lines. The face-on
maps exhibit multi-arm spiral-like features with cloud-like
high-density regions. Inhomogeneous structures are also
prominent from $\theta_v = 75^\circ$. In the following results, $\theta_v = 75^\circ$
which is suggested by comparing with the SED of the Circinus
galaxy (W16), is assumed, if not stated. Moreover, we notice
that most CO emissions originate from the disk region and,
furthermore, there are no dense axial “molecular winds”
outflow along the rotational axis. It would be interesting to
understand the origin of the kiloparsec-scale molecular out-
flows observed in nearby AGNs, such as NGC 1068 (García-
Burillo et al. 2014; see also discussion in Section 4.3).

In Figure 4, the changes in the intensity $I_v$, source function
$S_v$, and optical depth $\tau_v$ of CO ($3-2$) along two different rays

Figure 3. Same as Figure 2, but for $\theta_v = 75^\circ$, which is suggested from the fit with the infrared SED of the Circinus galaxy (W16).
toward the observer in a velocity channel ($\pm 2.5$ km s$^{-1}$ around the systematic velocity) are shown. Along the rays, the optical depth $\tau_v$ spatially changes by many orders of magnitude. There are several optically thick regions, which are non-uniformly distributed, and they form several discrete “clouds” along this sample line of sight (Figure 4(a)). The intensity increases from the background (i.e., CMB) at $y \sim 3 - 10$ pc, where $0.1 \lesssim \tau_v$, and is saturated at the clouds where $\tau_v > 1$ or stays constant if $\tau_v \ll 1$. At the observer side ($y \gtrsim 25$ pc), the intensity exceeds the source function and is therefore absorbed at the nearside grids depending on the local optical depth. A relatively optically thin case is also shown in Figure 4(b). The intensity increases following $\sim \tau_v S_0$ at the far side (i.e., $y \lesssim 10$ pc), and it is slightly absorbed at the nearside. This represents the characteristic feature of the line transfer effect through a highly non-uniform medium. It is then inferred that the observed integrated intensity in terms of the line-of-sight velocity does not necessarily represent a single state of the internal structure of the circumnuclear disk along a given line of sight (see also Section 3.4).

3.2. X-factor

Because it is difficult to directly observe emission from cold molecular hydrogen, the line intensity of CO (often $J = 1 \rightarrow 0$) is used to estimate the column density of H$_2$ in giant molecular clouds in our Galaxy, as well as the total molecular mass in external galaxies. The CO-to-H$_2$ conversion factor is often represented as $X_{\text{CO}}$ for the number density or $X_{\text{CO}}$ for the mass density. Based on various independent methods, it is estimated for the Galactic disk that $X_{\text{CO} (1-0)} \approx 2 \times 10^{20}$ cm$^{-2}$ (K km s$^{-1}$)$^{-1}$ or $\alpha_{\text{CO} (1-0)} = 4.3 M_\odot$ pc$^{-2}$ (K km s$^{-1}$)$^{-1}$, using the CO(1–0) intensity, and the error could be within a factor of 2–3 for molecular clouds in our Galaxy (Bolatto et al. 2013). Although this fiducial value is often also used for observations of external galaxies, it should not be the same in different environments, such as the ISM around AGNs or in starburst regions. Here, we present an independent estimate of the conversion factor using the line transfer calculations shown in Section 3.1. One should note that the values could be the case for the central region of the Circinus galaxy and could also be applied to low-luminosity AGNs associated with nuclear starbursts, but it is not necessarily the case for all types of AGNs, such as luminous quasars.

Figure 5 shows $X_{\text{CO}}$ (and $\alpha_{\text{CO}}$ for the right vertical axis) as a function of the line intensities of CO$(1-0)$, CO$(2-1)$, CO$(3-2)$, and CO$(4-3)$ based on the non-LTE line intensity calculations and H$_2$ density in the input data. It is apparent that the CO-to-H$_2$ conversion factor is not a constant and strongly depends on the line intensity, especially for the low-J lines. If we fit the conversion factor for $J = 1 \rightarrow 0$ with a single power law, we can obtain $X_{\text{CO} (1-0)} \approx 2 \times 10^{20}$ cm$^{-2}$ $(\text{K}$ cm s$^{-1})^{-1} - 10^{4.8}$ (K km s$^{-1}$)$^{-1}$, or $\alpha_{\text{CO} (1-0)} \approx 4.3 M_\odot$ $(\text{K}$ cm s$^{-1})^{-1} - 10^{4.8}$ (K km s$^{-1}$)$^{-1}$, where the integrated intensity $I_0 = 300$ K km s$^{-1}$. For $J = 3 \rightarrow 2$, $X_{\text{CO} (3-2)} \approx 2 \times 10^{21}$ cm$^{-2}$ $(\text{K}$ cm s$^{-1})^{-1} - 10^{4.8}$ (K km s$^{-1}$)$^{-1}$, or $\alpha_{\text{CO} (3-2)} \approx 44 M_\odot$ $(\text{K}$ cm s$^{-1})^{-1} - 10^{4.8}$ (K km s$^{-1}$)$^{-1}$, where the integrated intensity $I_0 = 300$ K km s$^{-1}$. Here, we assume $v_{\text{L}} = 10$ km s$^{-1}$ and $G_0 = 1000$. For other fitting results, see Table 1.$^9$

One should also note that the dispersion of $X_{\text{CO}}$ is more than one order of magnitude for a given intensity, which reflects the fact that the physical and chemical conditions are far from uniform in the circumnuclear disk and are also due to the effect of the line transfer in the inhomogeneous medium (Section 3.1

| Line   | $a$      | $b$      | $c$   | $d$   | $I_0$ |
|--------|----------|----------|-------|-------|-------|
| 1-0    | 2.0      | 4.8      | 4.4   | 4.8   | 600   |
| 1-0    | 2.5      | 1.5      | 5.5   | 1.5   | 300   |
| 2-1    | 15.8     | 7.4      | 34.4  | 7.4   | 600   |
| 2-1    | 5.0      | 1.3      | 10.9  | 1.3   | 300   |
| 3-2    | 20.0     | 3.0      | 44.0  | 3.0   | 300   |
| 3-2    | 4.0      | 0.5      | 8.7   | 0.5   | 100   |
| 4-3    | 200.0    | 4.3      | 436.0 | 4.3   | 300   |
| 4-3    | 12.6     | 0.9      | 27.5  | 0.9   | 100   |

Note. $I_0 \equiv 300$ (K km s$^{-1}$)$^{-1}$. The conversion factor in the intensity range of $I > I_0$ is fitted.
The strong positive dependence of the X-factor on the intensity implies that the lines are saturated with $I_S = n_S$ in optically thick, high-density clumps, which are more frequent along the line of sight in bright regions, as seen in Figure 4(a). These conditions in the ISM around the AGN are in contrast with the local GMCs or molecular gas in the disks of normal galaxies, where the X-factor is often assumed to be roughly constant.

We found that the X-factor does not strongly depend on the value of FUV ($G_0$) but tends to be smaller for larger $v_{\text{turb}}$ (see Figures 11(e) and (f), and the discussion in Section 4.2).

### 3.3. The CO Ladder

In Figure 6, we show the total integrated intensity of the CO lines as a function of the rotational transition number $J$, i.e., the SLED for the brightest spot and the intensity-weighted average value. Both show that the intensity with respect to CO(1–0) has a peak around $J = 6$. The SLED of the brightest spot is close to that for the gas in LTE with $T_{\text{gas}} = 20$ K (black dashed line). As shown by the weighted average (blue line) in the non-LTE case, most regions of the disk projected on the sky (see Figure 2) are not thermalized. This is because the internal structures of the disk are considerably clumpy and the line of sight is mostly occupied with optically thin gas (see Figure 4 and Section 3.1).

Note that if we assume LTE for all grid cells and calculate the line transfer, as for the non-LTE case, the resultant SLEDs (dashed blue and red lines) are very different. In a non-uniform medium with a large difference in optical depth, the LTE assumption in each grid cell does not necessarily cause the “observed” line ratios of the integrated intensities to be proportional to $v^2$. In the present case, the CO(1–0) becomes relatively weaker than CO(3–2) because of the line transfer effect; as a result, the line ratios appear “super-thermal.”

Zhang et al. (2014) showed the CO SLED using Atacama Pathfinder EXperiment (APEX) for the central 18" (~360 pc) of the Circinus galaxy and demonstrated that the observed $^{12}\text{CO}$ SLED has a maximum at $J = 5 - 6$. Using the large velocity gradient (LVG) approximation, they suggested that the gas density of H$_2$ is $10^{2.7-3.3}$ cm$^{-3}$, the temperature is 80–400 K, and the velocity gradient $dv/dr$ is 1–25 km s$^{-1}$ (assuming a uniform abundance of CO of $x_{\text{CO}} = 8 \times 10^{-5}$). As the radius of the observed region is 10 times larger than that of the present model, we cannot directly compare our model with this APEX result. Moreover, the abundance distribution of CO should not be uniform as suggested by our result (Figure 1(b)). However,
the suggested ranges of the physical conditions are consistent with those in the high-density gas in our numerical model.

3.4. Physical Conditions of the ISM Inferred from Line Ratios

Line ratios are often used to infer the physical states (e.g., density, temperature, and velocity dispersion or gradient) of the ISM in Galactic and extragalactic objects. For molecular lines, the numerical results with the LVG approximation or one-zone numerical code, such as RADEX (van der Tak et al. 2007), can be compared with the observed line ratios, taking the velocity gradient and fractional abundance as free parameters. In our 3D model, the physical conditions differ between grid cells on a scale of a few parsecs along the observed lines of sight; therefore, a specific observed line ratio does not necessarily represent a single physical state of the ISM.

In Figure 7(a), the line ratio (in Jansky) of $R_{32} \equiv J(\text{CO}\, 3\rightarrow 2)/J(\text{CO}\, 1\rightarrow 0)$ is plotted on a plane of the gas density and kinetic temperature derived from the input hydrodynamic data for the viewing angle of 90°. Only grid cells with $n_H > 0.1$ are plotted. This indicates that a line ratio could have been produced with more than three orders of magnitude in density. There is a weak tendency that $R_{32} \sim 5$ for higher-density gas ($n > 10^3 \text{ cm}^{-3}$) and $R_{32} \lesssim 3$ for lower-density gas ($n \lesssim 10^2 \text{ cm}^{-3}$). However, there are significant exceptions. The gas temperature is almost independent of $R_{32}$, except for the highest-density gas ($n > 10^4 \text{ cm}^{-3}$), where $R_{32} > 5$ and $T_{\text{kin}} \lesssim 50 \text{ K}$.

Figure 7(b) illustrates how the optical depth of CO($3\rightarrow 2$) depends on the H$_2$ density and $R_{32}$. In the optically thick grid cells, the gas density is $n > 10^4 \text{ cm}^{-3}$, where $R_{32} \sim 3$–6. Note that there is a small number of “super-thermal” grid cells where $R_{32} > 9$. These points do not necessarily indicate that the gas along its line of sight is excited non-thermally, but it is caused by the difference in the line transfer effect in different lines. Figures 8(a) and (b) are, in contrast, plotted against the local value of $R_{32}$, which is the line transfer effect over grid cells is not taken into account. The local density now corresponds more clearly than in the non-LTE case. Figure 8(b) shows that $R_{32} \sim 6.5$ for optically thick grid cells ($\tau_{\text{CO}\, 3\rightarrow 2} \gg 1$), where $n_{\text{H}_2} > 10^4 \text{ cm}^{-3}$ and $T_{\text{gas}} \sim 20 \text{ K}$. The ratio is expected for the gas in LTE. Most of the other grid cells are optically thin and not thermalized.

4. Discussion

In our numerical modeling, there are two free parameters that could affect the results, i.e., the velocity dispersion inside one
grid cell (i.e., micro-turbulence) and the strength of the FUV radiation. We discuss these effects below.

4.1. Effect of Microturbulence

The molecular line profile in our treatment is assumed to be a Gaussian profile with a dispersion \( v_{\text{turb}} \) originating from the unresolved internal turbulence in a grid cell. The relevant value of \( v_{\text{turb}} \) in the molecular clouds in external galaxies, especially under the influence of the AGN, is still not clear. One possible clue to estimate it is the size-dispersion relation of molecular clouds in the Galactic center. Tsuboi & Miyazaki (2012) suggested, using CS(1–0), that the velocity dispersion of molecular gas in the central molecular zone and in “50 km s\(^{-1}\) molecular clouds” is about five times larger for a given size than that in typical GMCs in the Galactic disk. This corresponds to \( v_{\text{turb}} \sim 7 \text{ km s}^{-1} \) for our grid size, i.e., 0.25 pc. As the nuclear region of the Circinus galaxy should be disturbed by intense feedback from the AGN, as well as from starbursts, in contrast to our Galactic center, the velocity dispersion on that scale could be larger than 10 km s\(^{-1}\).

Figure 9 shows the SLED, similar to Figure 6, but for the micro-turbulence \( v_{\text{turb}} = 1, 5, 10, 20, \) and 50 km s\(^{-1}\). Although the behavior of the intensity in terms of \( J \) is similarly independent of \( v_{\text{turb}} \), it shows that the intensity for a given \( J \) increases with \( v_{\text{turb}} \). This is because the optical depth is proportional to the line profile function \( q_0 \). Figure 10 presents the optical depth distribution for a given line of sight. It shows that for larger \( v_{\text{turb}} \), the intensity at the line center decreases, but the total integrated intensity increases because there are more regions with \( \tau_c > 0 \).\(^{10}\) The present results suggest that if we obtain the SLED in observations with a sufficiently fine spatial resolution (e.g., sub-parsec) for the central tens of parsecs in nearby AGNs, we could determine a relevant value of the micro-turbulence in the molecular clouds. This will be discussed in a subsequent paper (T. Izumi et al. 2018, in preparation).

Figure 10. Optical depth (CO(3–2)) distribution along a line of sight in four different models with varying internal turbulent velocities \( v_{\text{turb}} \), showing that the X-factor tends to be smaller for larger micro-turbulence values for a given line intensity. However, the dispersion does not significantly change among the results.

4.2. Effect of FUV

FUV field strength is one of the important quantities to determine the chemistry and thermal structures in the photo-dissociation region around central regions of galaxies (Meijerink & Spaans 2005; Wada et al. 2009). In starburst regions, the local value of the FUV should vary over several orders of magnitude (Rosenberg et al. 2014), e.g., \( G_0 = 100 \sim 10^3 \), depending on the local structures of the ISM and the distance to the radiation sources. Assuming the observed star formation rate (SFR) in the Circinus galaxy (Hicks et al. 2009), i.e., \( \sim 100 \, M_\odot \, \text{yr}^{-1} \, \text{kpc}^{-2} \), and the relation between \( G_0 \) and SFR density in the IR-luminous merger NGC 1614 (Saito et al. 2017), the FUV in Circinus can be estimated as \( G_0 = 10^2 \sim 10^3 \) on average (note that the scatter could be extremely large, ranging from \( G_0 = 10 \) to \( 10^6 \)).

If we directly solve the radiative transfer equations for the FUV in the inhomogeneous media with many radiation sources, our present model could be more realistic. However, this is beyond our current numerical treatment, so we assumed here a uniform \( G_0 \) and varied it as a free parameter. We confirm that the X-factor does not significantly depend on the strength of the uniform FUV between \( G_0 = 10^2 \) and \( 10^4 \) (Figures 11(e) and (f)), because both the intensity of CO and the molecular hydrogen density are similarly affected by the change in FUV (Wada et al. 2009).

4.3. Effect of the Viewing Angle and Implications on Other AGNs

Until now, we have focused on the case of edge-on views of the galaxy, which offer plausible explanations for the circum-nuclear disk in Circinus (Wada et al. 2016). However, it would be worth investigating how these results change for different viewing angles, in order to understand whether the present results are applicable to other AGNs. Figure 12 shows the SLED, X-factor, and \( R_{\ell q} \), for which the viewing angle \( \theta_v = 0 \) (i.e., face-on) is assumed. The SLED (Figure 12(a)) can be compared with Figure 6. The brightest spot (red solid line) in both cases is close to the LTE case with \( T_{\text{km}} = 20 \) K; however,
the intensity in the face-on case tends to be smaller, especially for high $J$. The weighted average value (blue solid line) does not depend on the viewing angle. The X-factor for CO ($3-2$) (Figure 12(b)) can be compared to that in Figure 5. Essentially, no significant difference was found in terms of the viewing angle between these two. The line ratio of CO ($3-2$)($R_{32}$) as a function of $T_{\text{kin}}$ and $n_H$ for the face-on view is plotted in Figure 12(c). Grid cells with $\tau > 0.01$ are plotted. For comparison, the same plot for the edge-on case is shown in Figure 12(d). Although the line ratio tends to be larger for a given density in the face-on case, as discussed in Section 3.4, it also exhibits a large dispersion in the gas density and temperature for a given line ratio. This is because the molecular gas forms a thick disk (Figure 1(a)), in which the internal structure on sub-parsec scales along the $z$-axis. If this inhomogeneous nature of the ISM in the central tens of parsecs exists in other AGNs, the results presented here should be interpreted in terms of the CO line observations.

Until now, the only “direct” detection of molecular lines from any known circumnuclear disk (CND) with a spatial resolution of a few parsecs is NGC 1068; this is the prototypical Seyfert 2 galaxy at $D = 14$ Mpc (García-Burillo et al. 2016). Using CO(6-5) line with ALMA, they claimed that the CND is a disk 7–10 pc in diameter, and it should be a counterpart of the “dusty torus,” as suggested by the near-IR and mid-IR interferometric observations (e.g., Jaffe et al. 2004). Although the spatial resolution ($\sim 4$ pc) is not sufficiently high to resolve sub-parsec inhomogeneous structures, the large velocity dispersion ($\sim 30$ km s$^{-1}$) and the lopsided distribution (i.e., $m = 1$ mode) imply the presence of complicated internal sub-structures, assuming that they do exist as found in our model for Circinus. In fact, the observed SED is well-fitted by a “clumpy” torus model (García-Burillo et al. 2016). However, our model disk for Circinus is globally axisymmetric, and no lopsided distribution of the molecular gas has been observed in contrast to NGC 1068. The condition for triggering the large-scale asymmetry is an interesting subject to be explored in terms of the hydrodynamic and magnetohydrodynamic instabilities, such as Papaloizou–Pringle instability (Papaloizou & Pringle 1984) and magnetorotational instability. The CO(6-5) observation of NGC 1068 shows no significant CO counterpart for the polar emission of the dust tori that are often seen in nearby AGNs (López-Gonzaga et al. 2016).
which is also the case in our “radiation-driven” fountain, where there is no dense molecular gas in the bipolar outflows.

The origin of sub-kiloparsec- to kiloparsec-scale molecular outflows/jets, such as in NGC 1068 (García-Burillo et al. 2014), Circinus (Zschaechner et al. 2016), and NGC 1377 (Aalto et al. 2016), and its physical link to the circumnuclear molecular gas remain unclear. The presence of 10 pc scale molecular outflows in NGC 1068 is under debate, even when certain distorted kinematics of molecular gas is observed in the torus (Gallimore et al. 2016). This is an interesting subject to be explored by high-resolution ALMA data of the central region of the Circinus galaxy, and will be discussed in a subsequent paper (T. Izumi et al. 2018, in preparation).

5. Conclusions

Recent observational and theoretical studies of obscuring material from sub-parsec to 100 pc scales around AGNs suggested non-static, multi-phase structures over wide density and temperature ranges. In this study, we calculated the line emissions from cold, molecular gas, which was expected in our previous “radiation-driven fountain model” (Wada et al. 2016). Using a snapshot of the 3D radiation-hydrodynamic simulation that reliably explains the SED of the nearest type 2 Seyfert galaxy, the Circinus galaxy, with XDR chemistry as an input, we conducted post-processed, 3D, non-LTE line transfer simulations for CO lines (J < 15) in the central r < 16 pc. We found that the CO emissions (J = 1–6) mostly originated from inhomogeneous structures. There are almost no “molecular outflows,” as the outflowing gas density is too low and mostly ionized. The SLED has a peak around J = 6 and its distribution suggests that the lines are optically thin for most regions. However, for a given line of sight, the optical depth distribution is highly non-uniform between τₜ < 1 and τₜ ≫ 1.

Because we know the molecular hydrogen density at each grid cell in the input model, we can obtain the CO-to-H₂ conversion factor (X_{CO} or α_{CO}). We found that the conversion factor depends strongly on the integrated intensity for a given line of sight, especially for lower J lines.
1. $X_{\text{CO}(1-0)} \approx 2.0 \times 10^{-20} \text{cm}^{-2} \left( \frac{I_{\text{CO}(1-0)}}{I_0} \right)^{1.8} \text{K km s}^{-1},$
2. $X_{\text{CO}(3-2)} \approx 2.0 \times 10^{12} \text{cm}^{-2} \left( \frac{I_{\text{CO}(3-2)}}{I_0} \right)^{3.0} \text{K km s}^{-1},$
3. $\alpha_{\text{CO}} \approx 4.4 M_\odot \left( \frac{I_{\text{CO}(1-0)}}{I_0} \right)^{4.8} \text{K km s}^{-1} \text{pc}^{-2},$
4. $\alpha_{\text{CO}} \approx 44 M_\odot \left( \frac{I_{\text{CO}(3-2)}}{I_0} \right)^{3.0} \text{K km s}^{-1} \text{pc}^{-2},$
5. $\alpha_{\text{CO}} \approx 300 \text{K km s}^{-1}$

One should note that there is large (more than one order of magnitude) scatter around this average value, reflecting the non-uniform internal structure (density, temperature, abundance, and velocity) of the “torus.” We also found that the conversion factor for a given intensity depends on the assumed value of the “micro-turbulence,” which is the velocity dispersion in one grid cell (0.25 pc in the present case). The values above could be the case for the central region of the Circinus galaxy, and they could also be applied to low-luminosity AGNs associated with nuclear starbursts, but not necessarily to all types of AGNs, such as luminous quasars.

The total CO intensities depend on the assumption of “micro-turbulence,” i.e., unresolved velocity dispersion inside a grid cell (0.25 pc). It is brighter for larger velocity dispersions (Figure 9), provided that $v_{\text{turb}} \lesssim 20 \text{ km s}^{-1}$. Using this fact, we can estimate the internal turbulent motion of the circumnuclear gas in Circinus and compare it with ALMA Cycle-4 observations of the central molecular disk (T. Izumi et al. 2018, in preparation).

We also found that the physical conditions differ between grid cells on a scale of a few parsecs along the observed lines of sight; therefore, a specific observed line ratio, such as $l_{\text{CO}(3-2)}/l_{\text{CO}(1-0)}$, does not necessarily represent a single physical state of the ISM. The dense ISM ($n > 10^4 \text{ cm}^{-3}$) on a 0.25 pc scale is mostly in a phase of molecules and LTE, but the resultant line ratio for an observer is not necessarily in LTE, because of the line transfer effect. These results basically do not depend on the choice of the viewing angle, as such, what we have discovered here could be useful in elucidating the physics of the ISM around supermassive BHs, not only in the Circinus galaxy, but also in other nearby AGNs. The present results also suggest that we need to carefully analyze the molecular line observations of the circumnuclear gas when we obtain them with a high spatial resolution in nearby AGNs by ALMA.

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ORCID iDs
Keiichi Wada @ https://orcid.org/0000-0002-8779-8486
Takuma Izumi @ https://orcid.org/0000-0001-9452-0813
Kohji Tomisaka @ https://orcid.org/0000-0003-2726-0892

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