Three-Dimensional Distribution of the ISM in the Milky Way Galaxy: IV. 3D Molecular Fraction and Galactic-Scale HI-to-H$_2$ Transition

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Abstract

Three dimensional (3D) distribution of the volume-density molecular fraction, defined by $f_{\text{mol}} = \rho_{\text{H}_2}/(\rho_{\text{HI}} + \rho_{\text{H}_2})$, is studied in the Milky Way Galaxy. The molecular front appears at galactocentric distance of $R = 8$ kpc, where the phase transition from atomic to molecular hydrogen occurs suddenly with $f_{\text{mol}}$ dropping from ~0.8 to 0.2 within a radial interval as narrow as ~0.5 kpc. The front in density $f_{\text{mol}}$ is much sharper than that for surface density molecular fraction. The front also appears in the vertical direction with a full width of the high-$f_{\text{mol}}$ disk to be ~100 pc. The radial and vertical $f_{\text{mol}}$ profiles, particularly the front behaviors, are well fitted by theoretical curves calculated using the observed density profile and assumed radiation field and metallicity with exponential gradients. The molecular fraction was found to be enhanced along the Perseus and some other spiral arms. The $f_{\text{mol}}$ arms imply that the molecular clouds are produced from HI gas in the spiral arms and are dissociated in the interarm region. We also show that there is a threshold HI density over which the gas is transformed into molecules.

Key words: galaxies: the Galaxy — galaxies: molecular gas — galaxies: hydrogen gas — ISM: molecules — ISM: hydrogen

1 INTRODUCTION

The atomic (HI) and molecular (H$_2$) hydrogen gases are the major constituents of the interstellar gas. The H$_2$ gas is dominant in the inner Galaxy, while HI in the outer Galaxy. The phase transition from HI to H$_2$ gases is determined by the environmental circumstances in the Galaxy such as the pressure or the density, radiation field and the metallicity. The molecular fraction, the ratio of molecular to total gas densities, is one of the fundamental quantities to represent the ISM conditions (Elmegreen 1993; Krumholz et al. 2009).

Galactic-scale variation of the molecular fraction has been studied in the Galaxy and nearby galaxies using HI and CO line observational data (Sofue et al. 1995; Honma et al 1995; Imamura and Sofue 1997; Hidaka and Sofue 2002; Nakanishi et al. 2006; Nakanishi and Sofue 2015; Tosaki et al. 2011; Tanaka et al. 2014). It was found that the molecular fraction is close to unity in the central regions, and decreases toward the outer galaxy. The transition of the gaseous phases from H$_2$ to HI occurs in a relatively narrow galactocentric region called the molecular front.

In the current studies, observational molecular fraction has been represented in terms of the surface densities (column densities) of HI and H$_2$ gases. In order to compare with the theoretical analyses, it is more appropriate to measure the quantities in terms of volume densities. In this paper we derive the volume-density molecular fraction in the Milky Way Galaxy, and investigate its three-dimensional distribution using the HI and H$_2$ density cubes obtained by Nakanishi and Sofue (2003,
2 3D Molecular Fraction

2.1 3D distributions of HI and H$_2$ gases

Figures 1 shows the distribution of surface (column) densities of HI and molecular gases projected on the galactic plane $\Sigma_{\text{HI}}$ and $\Sigma_{\text{H}_2}$, and figure 2 shows meridional cross section of the gas disk across the Galactic Center showing the volume densities $n_{\text{HI}}$ and $n_{\text{H}_2}$ in the $(X, Z)$ plane (Nakanishi and Sofue 2003, 2006, 2015). The molecular gas is distributed in a thin and dense disk near the galactic plane, embedded in the broader and more extended HI disk.

2.2 3D molecular fraction

The surface-density (column density) molecular fraction is defined by

$$f^\Sigma_{\text{mol}} = \frac{\Sigma_{\text{H}_2}}{\Sigma_{\text{HI}} + \Sigma_{\text{H}_2}} = \frac{2N_{\text{H}_2}}{N_{\text{HI}} + 2N_{\text{H}_2}},$$

where $\Sigma_{\text{HI}}$ and $\Sigma_{\text{H}_2}$ are the surface densities of neutral hydrogen and molecular gases, $N_{\text{HI}}$ and $N_{\text{H}_2}$ are the column densities, respectively, integrated in the direction perpendicular to the galactic plane.

The volume-density molecular fraction is defined by

$$f^\rho_{\text{mol}} = \frac{\rho_{\text{H}_2}}{\rho_{\text{HI}} + \rho_{\text{H}_2}} = \frac{2n_{\text{H}_2}}{n_{\text{HI}} + 2n_{\text{H}_2}},$$

where $\rho_{\text{HI}}$ and $\rho_{\text{H}_2}$ are the volume densities of the HI and molecular hydrogen gases, and $n_{\text{HI}}$ and $n_{\text{H}_2}$ are the volume number densities, respectively.

Using the data cubes for HI and H$_2$ gases derived by Nakanishi and Sofue (2015), we constructed a three dimensional cube of the surface- and volume-density molecular fraction $f^\Sigma_{\text{mol}}$ and $f^\rho_{\text{mol}}$. Figure 3 shows two dimensional distributions of the surface-density molecular fraction $f^\Sigma_{\text{mol}}$, and figure 4 shows volume-density molecular fraction $f^\rho_{\text{mol}}$ in the galactic plane at $Z = 0$. Figure 5 shows vertical cross section of the 3D $f^\rho_{\text{mol}}$ map at $Y = 0$. Figure 6 shows sliced maps of $f^\rho_{\text{mol}}$ distribution at different heights at every $\Delta Z = 40$ pc from $Z = -500$ pc to $+500$ pc.

Both figures 3 and 4 show that the high-molecular fraction region is located in the inner Galaxy at $R < \sim 8$ kpc, but the volume-density molecular fraction shows much clearer plateau-like distribution. The edge of the plateau is called the molecular front, where the galactic scale phase transition from HI to H$_2$ is occurring.

2.3 Radial molecular front

Figure 7(a) shows radial variations of the HI, H$_2$, and total gas densities in the galactic plane at $Z = 0$ kpc as a function of
the galacto-centric distance along the X axis ($Y = 0$). Figure 7(b) shows the corresponding volume-density molecular fraction $f_{\text{mol}}^\Sigma$. It shows also the surface-density molecular fraction $f_{\text{mol}}^\Sigma$ in the $(X, Z)$ plane calculated for the integrated column densities in $Z$ direction.

In the present analysis, we used densities along the $X$ axis at $Y = 0$ kpc, where kinematical distances, and therefore densities, are determined in much better accuracy than those along the $Y$ axis across the Sun, where the kinematical distance determination is most uncertain.

The volume-density molecular fraction is as high as $f_{\text{mol}} \sim 0.9$ at $R \leq 5$ kpc, and steeply decreases to low values less than 0.1 at $R > 9$ kpc with an $e$-folding radius interval of $\Delta R \sim 0.5$ kpc from $R = 7.5$ to 8 kpc. The figure indicates that the high molecular fraction region composes a plateau-like disk with critical radius $R_F \sim 8$ kpc, where the fraction decreases sharply with radius, which we call the front radii.

On the other hand, the surface-density molecular fraction varies smoothly with the maximum value of about $f_{\text{mol}}^\Sigma \sim 0.7$ at $R \leq 5$ kpc. Such a mild variation of $f_{\text{mol}}^\Sigma$ is due to averaging effect of the thicker HI disk having smaller molecular fraction at high $Z$ regions as seen in figure 2.

The distribution of $f_{\text{mol}}^\Sigma$ may be compared with those obtained for external galaxies: Similar front structure has been observed in nearby spiral galaxies (Sofue et al. 1995; Honma et al. 1997; Tanaka et al. 2014). A milder variation has been observed in later type galaxies like M33 (Tosaki et al. 2011), where the maximum fraction was found to be about $f_{\text{mol}}^\Sigma \sim 0.22$ at $R \sim 0.6$ kpc.

It should be emphasized that the volume-density molecular fraction obtained here in the Milky Way shows a much clearer, sharper front behavior than those ever observed for surface molecular fraction in galaxies.

### 2.4 Vertical molecular front

The 3D distribution of the molecular fraction makes it possible to examine the vertical variation of $f_{\text{mol}}^\Sigma$ in details. Figure 5 shows cross sections of the cube in $(X, Z)$ planes at different $Y$, and an enlarged map at $Y = 0$ across the Galactic Center.

Figure 8 shows vertical variations of $f_{\text{mol}}^\Sigma$ at different radii from $R = 0$ kpc at the Galactic Center to $R = 14$ kpc at $\Theta = 45^\circ$. This figure indicates that the galactic disk inside the solar circle, particularly at $\leq 5$ kpc, is molecular-gas dominant with...
Fig. 3. Surface density molecular fraction $f_{mol}$ in the $(X, Y)$ plane. Contour interval is 0.1. [Note: The straight radial features toward the bottom (also in figures 4 and 5) are artifacts due to edge-smoothing effect between data and blank regions.]

Fig. 4. Volume density molecular fraction $f_{mol}$ at $Z = 0$ kpc in the $(X, Y)$ plane. Contour interval is 0.1.

Fig. 5. $(X, Z)$ cross section of the 3D density molecular fraction $f_{mol}$ at $Y = 0$.

Fig. 7. (a) Radial variation $n_{HI}$ (dotted line), $2n_{H_2}$, and total density $n_{total}$ along the $X$ in the galactic plane ($Z = 0$ kpc) along the $X$ axis at $Y = 0$ kpc. (b) Radial variation of the volume-density molecular fraction $f_{mol}$ (thick line), compared with the surface-density molecular fraction $f_{mol}$ (thin line). The dashed line shows a calculated curve for the Elmegreen’s (1993) model using the code of Tanaka et al. (2014). See figure 10 and the text for details.
the cold neutral medium (CNM) from warm (WNM) phase. The value may represent a threshold ISM density to generate

\[ f_{\text{mol}}^p \sim 0.8 - 0.93 \text{ and as high as } \sim 0.5 \text{ even near the solar circle. It then drastically decreases outside the solar circle.} \]

It should be stressed that the \( f_{\text{mol}}^p \) decreases sharply with the height at \( \pm 50 \text{ pc} \) from the midplane of maximum \( f_{\text{mol}}^p \), exhibiting vertical molecular front of the molecular disk at \( h_c \sim \pm 50 \text{ pc} \). The shapes of the vertical and radial molecular fronts are similar except for the scale radius and height.

2.5 Threshold HI Density

It is known that the molecular gas is formed from and is dissociated into HI gas responding to the interstellar condition, and the molecular fraction is a function of the gas density through the pressure \( P = n_{\text{tot}} k T \) with \( T \) being the equivalent ISM temperature, the metallicity \( Z \), and the UV radiation field intensity \( j \) (Elmegreen 1993). We here examine the dependence of \( f_{\text{mol}}^p \) on the densities. Figure 9 plots \( f_{\text{mol}}^p \) against \( n_{\text{HI}} \), \( 2n_{\text{H}_2} \), and \( n_{\text{tot}} \).

The molecular fraction can be expressed by a simple function of the total and \( H_2 \) densities as

\[ f_{\text{mol}}^p = \frac{1}{1 + \eta^p} f_{\text{max}}, \]

where \( \eta \) is the ratio of the density to a critical density given by \( \eta = n(\text{H})/n_c \). We show the calculated function in the figure for the following parameters.

The dependence of \( f_{\text{mol}}^p \) on the total gas density is approximately represented by a parameter combination as \( f_{\text{max}} = 0.96 \), \( n_c = 7.0 \text{ H cm}^{-3} \), and \( b = -2.5 \), as shown by open circles in figure 9 and fitted by the dashed curve. The critical density of 7 H cm\(^{-3}\) is close to that of the molecular front in figure 7. The value may represent a threshold ISM density to generate the cold neutral medium (CNM) from warm (WNM) phase.

Similarly, \( f_{\text{mol}}^p \) depends on the molecular gas density by

\[ f_{\text{max}} = 1.0, n_c = 3.0 \text{ H cm}^{-3} \text{ and } b = -1.1, \]

as shown by the filled circles fitted by the thin full line.

On the other hand, the \( f_{\text{mol}}^p \) dependence on the HI density is quite different, showing rather an anti-correlation, so that \( f_{\text{mol}}^p \) decreases with increasing HI density. Also interestingly, \( f_{\text{mol}}^p \) drops suddenly at an HI threshold value of \( n_{\text{HI}} \simeq 3.5 \text{ H cm}^{-3} \). This implies that there is a maximum HI density, exceeding which the HI gas is transformed into molecular gas.

3 Comparison with Theoretical Models

The variation of \( f_{\text{mol}}^p \) in the \( R \) and \( Z \) directions can be calculated by a theoretical consideration of the phase transition in the interstellar gas taking account of the ISM pressure \( P \), metallicity \( Z \), and ultra-violet radiation (UV) field by stars \( j \) (Elmegreen 1993; Tanaka et al. 2014).

We consider two cases of pressure distribution. In the first model (Model 1), the pressure \( P \) is expressed by an exponential function, and in the second semi-analytical model (Model 2) we adopt the observed total density distribution along the \( X \) axis at \( Z = 0 \) and \( Y = 0 \text{ kpc} \) as shown in figure 7. This direction was chosen for accurate densities than those along \( Y \) axis (Sun-Galactic Center line), where the density is less certain for degenerated kinematic distances.

In Model 1 \( P \) is given by

\[ P = P_0 e^{-(r - R_0)/R_F}, \]

where the scale radius is taken to be \( R_F = 3 \text{ kpc} \). In Model
2, the pressure \( P \) is assumed to be proportional to the observed total hydrogen density as

\[
P = n_{\text{tot}} kT. \tag{5}
\]

We normalize the density by \( n_{\text{tot,0}} = 5.3 \text{ cm}^{-3} \) from the present measurement at \( R = X = 8 \text{ kpc} \) as an approximate representative value at the Sun. The temperature is assumed to be constant at \( T = 7000 \text{ K} \), equivalent to the velocity dispersion of clouds and interstellar turbulence, which is close to the pressure-equilibrium kinematic temperature, 8000 K, of the warm neutral medium (Heiles and Troland 2003). Here and hereafter, the suffix 0 denotes the values at \( R = 8 \text{ kpc} \) approximately representing the solar value.

In both models, we adopt the same profiles for \( j \) and \( Z \) as

\[
j = j_0 e^{-(R-R_0)/R_j} \tag{6}
\]

and

\[
Z = Z_0 e^{-(R-R_0)/R_Z}. \tag{7}
\]

The radiation field is assumed to have the same scale radius as the pressure, \( R_j = 3 \text{ kpc} \), and the solar value (Allen 1973) is the same as taken by Elmegreen (1993).

The scale radius of the metallicity distribution was determined by Shaver et al. (1983), who obtained a radial gradient as \( d \log Z / dR = -0.07 \pm 0.015 \text{ dex kpc}^{-1} \) for \( R_0 = 10 \text{ kpc} \), which corresponds to \(-0.088 \pm 0.019 \text{ dex kpc}^{-1} \) for \( R_0 = 8 \text{ kpc} \). This yields \( Z = Z_0 e^{-(R-4.93 \pm 1.1 \text{ kpc})} \), and we assume \( R_Z = 4.93 \text{ kpc} \).

Calculated results for the two models are shown in figures 7 and 10. The exponential model (Model 1) shows smooth and mild variation. Although it roughly approximates the general behavior of observed \( f^{\text{mol}}_m \), the sharp molecular front cannot be reproduced. On the other hand, the semi-analytical model (Model 2) using the observed density profile well reproduces the observed \( f^{\text{mol}}_m \), when the ISM temperature is taken to be 7000 K. The model can reproduce not only the steep molecular front at \( R \approx 8 \text{ kpc} \) but also the fluctuations.

The model profile is sensitive to the ISM temperature. If the temperature is changed to \( \sim 10^5 \text{ K} \) or to \( \sim 5000 \text{ K} \), the fitting gets worse, with \( f^{\text{mol}}_m \) being increased or decreased significantly, as shown in figure 10(c). This implies that the \( f^{\text{mol}}_m \) fitting can be used to determine the ISM temperature, if the radiation field and metallicity are given.

The \( Z \) directional density profile is expressed by a hyperbolic cosecant function of the height \( Z \). The metallicity and the radiation intensity field are expressed by an exponentially decreasing function with \( R \) and \( Z \). The \( Z \)-directional variation of model \( f^{\text{mol}}_m \) is shown in figure 8 for the inner region of the Galaxy. The steep vertical variation of \( f^{\text{mol}}_m \) near the vertical molecular front is well reproduced by this model.

### 4 Spiral Arms

In order to see the variation of molecular fraction in relation to the spiral arms, we made unsharp-masked (background filtered) map of the density molecular fraction at the galactic plane. Figure 11 shows unsharp-masked images of the total gas density and molecular fraction. In the figure the spiral arms traced in our earlier works (Nakanishi and Sofue 2006, 2015) are superposed.

The unsharp-masked \( f^{\text{mol}}_m \) map shows spiral arm structure similar to that in the total gas arms. A clear correlation is found in the Perseus Arm, where the \( f^{\text{mol}}_m \) arm almost perfectly traces the spiral arm. Similar correlation, though not so clear as in Perseus, is also found along the Scutum, Sgr, and outer arms.

The enhancement of the molecular fraction along the spiral arms implies that the molecular clouds are produced inside the arms, and are dissociated when the clouds go out into the interarm. Formation of molecular gas inside the spiral arms is
more efficient in regions outside the solar circle with smaller molecular fraction than in the inner regions with almost saturated fraction. Namely, the \( f_{\text{mol}}^{\text{rot}} \) arms are more apparent in the transition regions, while they are not clearly visible in the innermost regions where the gas is already nearly molecular.

Thus, we may conclude that the molecular gas is produced in the spiral arms at \( R \sim 10 \) kpc. This is consistent with the long arm-interarm crossing time of the spiral pattern near the Perseus arm on the order of

\[
t \sim \pi/(\Omega - \Omega_{\text{p}}),
\]

which is on the order of \( \sim 10^9 \) yrs and is sufficiently longer than the molecular gas formation time scale \( t_{\text{mol}}^{\text{rot}} \sim 10^7 \) yrs (Goldsmith et al. 2007). Here, \( \Omega = V_{\text{rot}}/R \sim 20 \text{km cm}^{-1}\text{kpc}^{-1} \) is the angular velocity of the disk gas for \( V_{\text{rot}} = 220 \text{ km s}^{-1} \) and \( R = 10 \) kpc, and \( \Omega_{\text{p}} \sim 23 \text{ km cm}^{-1}\text{kpc}^{-1} \) (Junqueira et al. 2015) is the pattern speed.

Note that there is a peculiar region near \((X, Y) \sim (-5, +5)\) kpc between the Scutum-Crux and Sagittarius-Carina Arms, where \( f_{\text{mol}}^{\text{rot}} \) runs along the interarm region. However, this is due to the sharp edge of the molecular front in this area which caused an artifact of arm-like enhancement when the unsharp-masking was applied.

5 Summary and Discussion

We constructed a 3D cube of the volume-density molecular fraction, \( f_{\text{mol}}^{\text{rot}} \), using the HI and H\(_2\) density cubes of the Milky Way. The radial molecular front in the galactic plane observed in the density molecular fraction \( f_{\text{mol}}^{\text{rot}} \) is found to be sharper than that for the surface density molecular fraction \( f_{\text{mol}}^{\Sigma} \). The molecular front is also found in the vertical distribution of \( f_{\text{mol}}^{\text{rot}} \).

Plots of \( f_{\text{mol}}^{\text{rot}} \) against HI, H\(_2\), and total gas densities showed that \( f_{\text{mol}}^{\text{rot}} \) is a function of the H\(_2\) and total gas densities empirically expressed by equation 3. A threshold value was obtained in the HI density at \( n_{\text{HI}} \simeq 3.5 \)HI cm\(^{-3}\), above which the gas is transformed almost totally into molecular gas.

The radial and Z-directional variations of the observed \( f_{\text{mol}}^{\text{rot}} \) and sharp molecular fronts are well reproduced by the simple model calculations. We showed that the radial profile is a sensitive function of the assumed ISM temperature, which was here taken to be 7000 K for reasonable fitting. The temperature is consistent with the pressure-equilibrium kinetic temperature, 8000 K, of the warm neutral medium (Heiles and Troland 2003).

The radial \( f_{\text{mol}}^{\text{rot}} \) profile was analyzed only along \(+Y\) axis for the highest quality of data in this direction as indicated from figures 1 and 4. The profile may represent the typical radial variation in the whole galaxy, and analyses along other radial directions will give almost the same result. Also, azimuthal averaging was not applied, as it smeared out the molecular fronts to be studied in this paper due to the globally asymmetric distribution of the gases (figure 1).

Two dimensional unsharp-masked (background-filtered) \( f_{\text{mol}}^{\text{rot}} \) map in the galactic plane exhibits spiral arms with enhanced molecular fraction. Most of the \( f_{\text{mol}}^{\text{rot}} \) arms correspond to the known spiral arms such as the Perseus arm. This fact implies that HI gas is transformed into molecular gas along the spiral arms with marginal \( f_{\text{mol}}^{\text{rot}} \) values, which occur at \( R \sim 8 \) kpc. Such spiral enhancement of \( f_{\text{mol}}^{\Sigma} \) has been also observed in the outer spiral arms of the spiral galaxy M51 (Hidaka and Sofue 2002).

Finally we comment on possible effects of the existence of cold and optically thick HI gases, which were not taken into account in the present analysis. In our analysis, the HI gas density was calculated for the usual conversion factor on the assumption that the HI line is optically thin. This assumption underestimates the HI densities, as the cold and optically thick HI gas mainly included in dense molecular clouds has been neglected.

We here consider possible effects of cold HI component. The existence of cold HI would increase the total HI density by a factor of \( \sim 2 \) (e.g., Fukui et al. 2015). This may decrease the \( f_{\text{mol}}^{\text{rot}} \) values in outer Galaxy, where the molecular gas is relatively rare, however, it will not be changed significantly in the inner Galaxy, where the HI density is negligible or much smaller than the molecular gas density. Accordingly, the molecular front may be slightly shifted toward inside, and hence, the \( f_{\text{mol}}^{\text{rot}} \) plateau in figures 4 and 8 will shrink slightly.

An \( f_{\text{mol}}^{\text{rot}} \) analysis taking account of the cold HI component will be a subject for the future.

References


Imamura, K, Sofue, Y., 1997, AA, 319, 1

Junqueira, T. C., Chiappini, C., Lépine, J. R. D., Minchev, I., & Santiago, B. X. 2015, MNras, 449, 2336


Nakanishi, H., Sofue, Y. 2003, PASJ, 55, 191


Fig. 11. Unsharp-masked total surface density (HI+2H\textsubscript{2}) map (top), and unsharp-masked \( f'_{mol} \) map for \( \Delta f'_{mol} \) (bottom). Contour interval is 0.02. Spiral arms traced by Nakanishi and Sofue (2015) are indicated by full lines. The radial patterns at the edges of blank and data regions are artifact during the unsharp-masking procedure.