Molecular cloud formation as seen in synthetic H\textsc{i} and molecular gas observations

Jonathan S. Heiner\textsuperscript{1}\textsuperscript{\star}, Enrique Vázquez-Semadeni\textsuperscript{1}, Javier Ballesteros-Paredes\textsuperscript{1}

\textsuperscript{1}Centro de Radioastronomía y Astrofísica (CRyA), Universidad Nacional Autónoma de México, C.P. 58190 Morelia, Michoacán, Mexico

Draft of 26 March 2014

ABSTRACT

We present synthetic H\textsc{i} and CO observations of a numerical simulation of decaying turbulence in the thermally bistable neutral medium. We first present the simulation, which produces a clumpy medium, with clouds initially consisting of clustered clumps. Self-gravity causes these clump clusters to merge and form more homogeneous dense clouds. We apply a simple radiative transfer algorithm, throwing rays in many directions from each cell, and defining every cell with $\langle A_v \rangle > 1$ as molecular. We then produce maps of H\textsc{i}, CO-free molecular gas, and CO, and investigate the following aspects: i) The spatial distribution of the warm, cold, and molecular gas, finding the well-known layered structure, with molecular gas being surrounded by cold H\textsc{i} and this in turn being surrounded by warm H\textsc{i}. ii) The velocity of the various components, finding that the atomic gas is generally flowing towards the molecular gas, and that this motion is reflected in the frequently observed bimodal shape of the H\textsc{i} profiles. This conclusion is, however, tentative, because we do not include feedback that may produce H\textsc{i} gas receding from molecular regions. iii) The production of H\textsc{i} self-absorption (HISA) profiles, and the correlation of HISA with molecular gas. In particular, we test the suggestion of using the second derivative of the brightness temperature H\textsc{i} profile to trace HISA and molecular gas, finding significant limitations. On a scale of several parsecs, some agreement is obtained between this technique and actual HISA, as well as a correlation between HISA and the molecular gas column density. This correlation, however, quickly deteriorates towards sub-parsec scales. iv) The column density PDFs of the actual H\textsc{i} gas and those recovered from the H\textsc{i} line profiles, finding that the latter have a cutoff at column densities where the gas becomes optically thick, thus missing the contribution from the HISA-producing gas. We also find that the power-law tail typical of gravitational contraction is only observed in the molecular gas, and that, before the power-law tail develops in the total gas density PDF, no CO is yet present, reinforcing the notion that gravitational contraction is needed to produce this component.

Key words: turbulence – ISM: clouds – ISM: evolution – ISM: kinematic and dynamics – ISM: structure

1 INTRODUCTION

The present view of the interstellar medium (ISM) is that it is in general highly turbulent (e.g., Vázquez-Semadeni et al. 2000, Mac Low & Klessen 2004, Elmegreen & Scalo 2004, Ballesteros-Paredes & Hartmann 2007), and that dense, cold clouds form where turbulent compressions or larger-scale instabilities produce converging flows that in turn cause the density to increase locally (e.g., Dobbs et al. 2014, Molinari et al. 2014). Indeed, numerical simulations of converging flows in the warm neutral medium (WNM) including self-gravity but no stellar feedback (Vázquez-Semadeni et al. 2007, 2011, Hennebelle et al. 2008, Heitsch & Hartmann 2008, Heitsch et al. 2009, Banerjee et al. 2009a) show in general that, once a dense cloud is formed by this mechanism, it quickly becomes gravitationally unstable, and begins to undergo gravitational collapse. An important feature of this collapse is that it begins in gas that should be primarily atomic, with molecule formation occurring as a consequence of the gravitational contraction, as initially proposed on theoretical grounds by Franco & Cox (1986) and Hartmann et al. (2001). Simulations including a self-consistent treat-
Figure 1. Three-dimensional distribution of the atomic density (green) and the molecular density (red) at the three timesteps through iso-surface renderings made with Starlink’s GAIA (see e.g. Draper et al. 2007). Two green intensity levels were used, of 1 and 3, 1.5 and 3, and 1.5 and 3 $M_\odot$ pc$^{-3}$, for the timesteps at 12.5, 25.0, and 33.7 Myr, respectively. Similarly, red levels of 0.44 and 13, 0.44 and 50, and 0.44 and 50 $M_\odot$ pc$^{-3}$, were respectively used at each of the timesteps to image the molecular gas density. The numbered axes correspond to the x, y and z axes respectively (with the x-axis pointing towards the lower left corner. A color version this figure is available in the online version of this journal.
direction of the motions that produce GMCs is a formidable
problem, due to the confusion caused by the ubiquitous pres-
ence of HI gas in the Galactic disk.

Several studies have been conducted to determine the
signatures in line profiles and position-velocity (PV) space
arising from the density and velocity features produced in
the simulations. Early studies simply investigated line-of-
sight (LOS) projections of the density field from numeri-
cal simulations, and perhaps investigated the column den-
sity in the velocity coordinate (line profiles and channel
maps) (e.g., Ballesteros-Paredes et al. 1999, Pichardo et al.
2009, Ostriker et al. 2001, Ballesteros-Paredes & Mac Low
2002), although without performing synthetic observations
based on integration of the radiative transfer (RT) equa-
tion for the various lines involved. A further step was made
by Ballesteros-Paredes & Mac Low (2002), who, in order to
study the internal structure of molecular clouds, created syn-
thetic CO and CS line profiles in local thermal equilibrium
from numerical simulations of isothermal molecular clouds.
They found that the density-size relation, rather than an
intrinsic property of molecular clouds, is an artifact of the
observational procedure (see also Ballesteros-Paredes et al.
2002), although without performing synthetic observations
in order to classify the gas as either being atomic or molec-
ular, and then investigate various aspects, such as the spa-
tial and spectral features was developed by Gibson &
Goldsmith (2000). Since strictly speaking we do not re-
quire molecular (CO) emission in order to identify HI self-
absorption, we will refer to these features as HISA regard-
less of whether they may be considered ‘normal’, as a matter
of convenience.

In general, HI profiles typically look bi-modal on or near
molecular clouds and it can be hard to distinguish without
additional information what physical properties are behind
this profile shape. In this contribution we therefore also aim
to explore the extent to which we can distinguish true HISA
from separate emission peaks, and how well the HISA is cor-
related with the presence of molecular gas at various evolu-
tionary stages of the clouds.

This paper is structured as follows: First, we introduce
the simulation and the synthetic observations derived from
it in Sec. 2 and discuss the density and velocity structure of
the various gas components in real space, emphasizing the
general trend of inflow onto the dense gas in Sec. 3. Then,
in Sec. 4 we discuss the nature of the synthetic line profiles,
and in Sec. 5 we address the identification of HISA features
and compare these features to those of the molecular gas.
Next, we discuss the structure of the probability density
functions of the simulation and the structure of the gas in
the context of colliding gas flows. In Sec. 6 we close with a
brief discussion and summary of our results.

2 THE METHOD

2.1 The numerical simulation

Our numerical simulation was performed using the GADGET-
2 code (Springel et al. 2001), with 296^6 \approx 2.6 \times 10^7 SPH
particles, and including prescriptions for sink particles taken
from Jappsen et al. (2005) and for heating and cooling from
Vázquez-Semadeni et al. (2007). The initial density and tem-
perature of the simulation were set at 3 cm^{-3} and 730 K, re-
spectively, representing the mean ISM conditions at a spiral
arm. The physical size of the numerical domain was 256 pc.
The simulation was started by applying a Fourier turbulence

© 201X RAS, MNRAS 000, 1–21
Figure 2. Slices of the atomic and molecular mass density (contours and grayscale respectively) in units of the simulation are displayed. The coordinates are in parsec offset with respect to one corner of the simulation cube. The atomic density contour levels are 0.1, 10 and $100 M_\odot pc^{-3}$ (the native units of the simulation) with the lowest contour colored gray.

driver with purely solenoidal modes between wavenumbers $k = 1$ and $k = 4$ for 0.65 Myr, reaching a maximum velocity dispersion of $\sigma \approx 18$ km s$^{-1}$ at $t \approx 0.65$ Myr.

For the analyses presented in this paper, we consider three timesteps of the simulation, at 12.5, 25.0 and 33.7 Myr, where the latter is the final recorded timestep of this simulation. An octant of the simulation, of size 128 pc per side, containing the most massive clouds, was interpolated onto a $256^3$ uniform grid, giving an effective resolution of 0.5 pc. This resolution was chosen to provide a resolution comparable to observations of the interstellar medium in our Galaxy, while allowing easy manipulation of the data. Within this 128 parsec$^3$ sub-volume, we focus on the entire sub-volume as well as on a further zoomed-in volume containing a dominant cloud feature (not necessarily the same cloud at each timestep). Images of the sub-volume at the three timesteps, after applying the RT prescription (cf. Sec. 2.2) are shown in Fig. 1.

2.2 Producing molecular gas

Once the data has been gridded, we proceed to distinguish between ‘atomic’ and ‘molecular’ gas. Note that the version of GADGET-2 that we use does not solve the chemistry explicitly, and so we use the simple criterion proposed by Heitsch & Hartmann (2008) for deciding which grid cell in the simulation are ‘atomic’ and which are ‘molecular’. While obviously faster than solving a full chemical network (e.g., Koyama & Inutsuka 2000; Clark et al. 2012), this prescription is rather approximative, in particular because it assumes that molecules form as soon as the physical conditions allow for it, rather than following the time-dependent process of molecule formation. Thus, our results should be considered as providing upper limits for the amount of molecular gas present in the simulation.

The prescription we use is as follows: from each grid cell we emit 100 rays in random directions, that reach out to the edge of the numerical box, and compute the column density along each ray. The column density is converted to a visual extinction $A_v$ using the standard formula $A_v \approx 10^{-21} N_H$. We then compute the average extinction $\langle A_v \rangle$ for each cell. If $\langle A_v \rangle > 1$ and $T < 50$K for a cell, we label its contents as
molecular, meaning hydrogen is in the form of H$_2$ molecules. If, in addition to satisfying the condition $\langle A_v \rangle > 1$, the density in the cell satisfies the local condition $n_{H_2} \geq n_{crit}$, then we assume that the cell contains CO molecules, with a fixed relative abundance of CO(1-0) to total molecular gas number density of $\sim 2 \times 10^{-4}$ (e.g. Cernicharo & Bachiller 1984). Pineda et al. (2008). The critical density is given by

$$n_{crit} \approx \frac{A_{ji}}{\sigma_{CO} \times \langle n_{H_2} \rangle},$$

(1)

where $A_{ji}$ is the Einstein A, $\sigma_{CO}$ is the collisional cross section of the CO(1-0) molecule (ignoring higher transitions), and $\langle n_{H_2} \rangle \approx 9.09 \times 10^3 \times \sqrt{T}$. The local gas temperature is available from the simulations at each resolution element. See Sect. 4 for further discussion.

An immediate implication of this procedure is that in our simulation, atomic and molecular gas are not mixed in a grid cell, which is either fully atomic, or fully molecular. Nevertheless, we can have mixing of atomic and molecular gas at scales larger than the grid cell size, if neighboring cells are in some cases atomic, and in other cases molecular. Therefore, it is perfectly feasible to have mixing of atomic and molecular gas along an observational line of sight although, as mentioned above, the molecular fraction we estimate will be an upper limit. In particular, we aim to investigate atomic gas that is about to turn molecular, and we expect our results, as they relate to H$_2$ self-absorption and atomic-to-molecular conversion, to provide us with an informative, albeit only approximate, view. Note also that, since we distinguish between atomic and molecular gas by post-processing of the simulation data, this distinction has no effect on the evolution of the simulation. We plot the three-dimensional distribution of the atomic and the molecular gas qualitatively in Figure 1.

Finally, we note that, because our simulation does not include stellar feedback, the conversion of atomic gas into molecular gas and finally into stars is essentially a one-way process, although potentially molecular gas may become atomic again if the local $A_v$ drops below unity or if the temperature rises sufficiently. We have not traced individual particles, so whether, or to what extent, this occurred in our simulation is unknown. No photodissociation physics were included.

3 GENERAL MORPHOLOGY AND COLD GAS FRACTION

As time progresses in the simulation, filaments and clumps of gas begin to form by gravitational contraction onto the density peaks produced by the initial turbulence, aided by the thermal instability (Ballesteros-Paredes et al. 1999; Vázquez-Semadeni et al. 2007, 2009; Heitsch & Hartmann 2008; Heitsch et al. 2009b; Banerjee et al. 2009; Gomez & Vázquez-Semadeni 2013). Figure 2 shows slices through the mass density cubes of the atomic and molecular gas, zoomed in to show example molecular cloud structures. Molecular clouds are formed in filament-like structures before collapsing. The positions in parsecs refer to the offset from the (0,0,0) coordinate at one corner of the gridded cubes.

In Figure 3, for the same zoomed-in areas in the three timesteps, we show the velocity field in the $(y, z)$ direction and the gas temperature. As expected, comparing this figure with Figure 2 the low density gas has a high temperature (the equivalent of the warm neutral medium), while denser gas is cooler, and eventually turns molecular. However, it is also noticeable that there are cold H$_2$ envelopes around the molecular gas.

In Table 1 we give the total, atomic, and molecular masses in the gridded volume as well as in the zoomed-in areas for the three times we study. It can be seen that the molecular mass fraction increases rapidly and that the velocity dispersion in the simulation decreases over time. The average density of the gridded volume increases slowly, namely 3.0, 3.5 and 4.1 cm$^{-3}$ at each timestep respectively, where 3.0 cm$^{-3}$ is also the average density of the full simulation volume. The increasing gas mass and density indicate that gas is flowing into the gridded volume, which was selected for its developing molecular cloud structures. This fact is also suggestive of gravitational contraction at the largest scales we are considering.

It is also instructive to compute the fraction of cold atomic gas in our simulation. This cold atomic gas exists when the local $A_v$ has not reached unity, at which point it would be deemed molecular. Krčo & Goldsmith (2010) found in their observational survey of molecular cores an abundance of cold H$_2$ column density to total proton column density of $10^{-2.8}$ or $\approx 0.0016$. In our simulation, we have computed the mass of cold H$_2$ (being cooler than 50 K and having $A_v$ below unity) versus the total gas mass, finding ratios of 0.00014, 0.00055 and 0.00027 respectively for our three increasing timesteps, or consistently between half and one order of magnitude less than the values Krčo & Goldsmith (2010) found. This is probably a consequence of our ‘instantaneous molecule formation’ assumption which, as mentioned above, causes our molecular gas fractions to be upper limits. Also, this ratio can vary due to molecular clouds forming in a non-continuous fashion and due to gas entering and leaving the sub-volume of the simulation that we selected.

4 SYNTHETIC H$_2$ AND CO PROFILES

4.1 Generation of the ‘observations’

One of the main goals of this contribution is to focus on the ‘observer’s perspective’. To this end, we derive H$_2$ and CO line profiles. In order to perform the 21-cm H$_2$ and CO(1-0) line profiles, we have assumed that both lines are in local thermodynamic equilibrium (LTE) for the population of the atom/molecule energy levels. This is a good approximation for the study of H$_2$ profiles, since H$_2$ clouds are dominated by collisions. In the case of molecular clouds, LTE is a reasonably good approximation to study the CO lines qualitatively, if the volume density is above a certain excitation threshold (Rohlfis & Wilson 1996). Since we know the detailed velocity, density and temperature fields, we have integrated the transfer equation along the line of sight, assuming that every pixel above the threshold has a blackbody emission at the corresponding temperature. The details can be found in Ballesteros-Paredes & Mac Low (2002). Here we just note that the H$_2$ emission will come from every resolution element that is not
Figure 3. Velocity of the gas in the y, z plane (arrows) and the temperature of the gas is plotted. We assume that cold gas (below 50K) with a local visual extinction above 1 has turned molecular. It can be seen that the gas is flowing into the cold areas.

Figure 4. Atomic hydrogen column density maps at the three timesteps. The rectangles mark the regions featured in subsequent figures (when not considering the full area). The white contours represent molecular gas column densities of $3 \times 10^{20}$, $5 \times 10^{20}$, and $10 \times 10^{20}$ cm$^{-2}$, respectively, in each of the timesteps.
deemed to be molecular, while the CO emission will come from molecular resolution elements \((A_v \geq 1 \text{ and } T < 50 \text{ K})\) as well as having a number density above the local critical density, in order to avoid including molecules that are under-excited (Roberts & Wilson 1996).

With this information, we can observe cold atomic gas as it is about to turn molecular. Even though atomic and molecular gas do not mix within individual cells in our synthetic observations, it can still appear that cold atomic gas coincides with molecular cores along a line of sight, if the cold atomic gas is either directly in front or behind the molecular gas. Because of this, our synthetic profiles should still look realistic, as long as they include a significant number of grid cells, which is generally the case. Note that, throughout this work, we use a velocity range of -15 to 15 km s\(^{-1}\) and a velocity spacing of 0.15 km s\(^{-1}\).

For simplicity, we choose the line-of-sight direction along the z-axis. Due to the randomness of the initial condition, there is no preferred direction and for our purposes it was unnecessary to specifically select clouds and produce synthetic line profiles along specific cloud axes. We leave those specific cuts for more specific future applications.

The CO line profiles were derived under the assumption that the ratio of the CO(1-0) to total molecular gas number density is (rather approximately) \(2 \times 10^{-4}\) (e.g. Cernicharo & Bachiller 1984; Pineda et al. 2008). In our case, varying the exact CO abundance leads only to a scaling effect in the line profiles, which in turn does not influence the morphology of the gas overall. Since we have not computed any actual chemical reactions, no further effects of the CO abundance exist in our simulation.

It is important to note that the critical density of molecular hydrogen is determined by the local temperature. Thus, a drawback of our approach is that we may miss some CO emission due to the limited resolution of the gridded volume, implying that we may be smoothing out a potentially clumpy medium. For example, if we have a molecular hydrogen density of 50 cm\(^{-3}\) with our standard grid cell size of (0.5 pc), and thus would not be labeled as CO by our procedure. However, it is possible that this gas was all concentrated in a volume of (0.23 pc)\(^3\) in the original SPH data cube, thus having a density of 500 cm\(^{-3}\), which, depending on the temperature, would already be quite close to the critical density for CO emission to occur, and therefore should be labeled as CO.

We will distinguish between column densities derived from the simulation directly and the inferred ‘observational’ column densities. The former are derived directly from the mass density cube by integration along the LOS (which is 128 pc), assuming a mean particle mass of \(m = 1.27\) for the calculation of \(N_{\text{atom}}\), and \(\mu = 2.36\) for \(N_{\text{mol}}\). On the other hand, for the HI and CO brightness temperature profiles we also produce velocity-integrated maps of \(N_{\text{HI}}\) (cm\(^{-2}\)) and \(W_{\text{CO}}\) (K km s\(^{-1}\)) respectively. These are the ‘observational’ quantities. It should be noted that \(W_{\text{CO}}\) is only calculated to provide a familiar quantity and is not meant to predict any absolute values, as no distance to the simulation volume was used or any kind of telescope resolution effects. The HI column density was computed from the HI brightness temperature profile using the common assumption of the atomic gas being optically thin.

### 4.2 Analysis of the profiles

Figure 4 shows the integrated HI column densities at our three timesteps and selection boxes (white rectangles) highlighting regions of interest because of the presence of molecular cloud structure. Extended gas structures are visible at a level of about 30 cm\(^{-2}\), permeating the entire 128-pc gridded volume. Our volume contains a large underdense region (below 1 cm\(^{-3}\)) that persists throughout our three timesteps under consideration, surrounding the dense, evolving dense clouds.

It is remarkable that, in spite of the obvious constraints and limitations of the simulation, there is a striking resemblance to the Taurus molecular cloud and its immediate surroundings in the first timestep (Figure 5). The region contains a molecular cloud in the upper left hand side, next to something that appears to be a cavity in the HI gas, surrounded by a diagonal band of HI. This type of structure could be labeled as an HI (super-)shell, although our simulations do not include the kind of supernova feedback that might produce HI supershells. We merely point out the resemblance to caution that the 2D projection of the atomic gas may look like a supershell, but further kinematic confirmation should be sought.

Figure 6 shows a zoom into the selection box of the 25-Myr timestep, showing HI brightness temperature profiles at various locations. The HI profiles almost universally show a depression around the zero-offset velocity. This depression may be caused either by a lack of atomic gas or by self-absorption. It is hard to determine from the observations alone which of these possibilities is the actual cause of the dip in the profile, but in the rest of this contribution we

### Table 1. Masses and velocity dispersions in both the gridded volume and the zoomed-in regions.

| Time       | \(M_{\text{tot}}\) (\(M_\odot\)) | \(M_{\text{atom}}\) (\(M_\odot\)) | \(M_{\text{mol}}\) (\(M_\odot\)) | \(\sigma_{v,\text{tot}}\) (km s\(^{-1}\)) | \(\sigma_{v,\text{atom}}\) (km s\(^{-1}\)) | \(\sigma_{v,\text{mol}}\) (km s\(^{-1}\)) |
|------------|-------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 12.5 (full)| \(2.0 \times 10^3\)           | \(1.9 \times 10^3\)            | \(9.2 \times 10^3\)            | 4.5                             | 4.5                             | 0.23                            |
| (sub-region)| \(4.2 \times 10^4\)           | \(3.8 \times 10^4\)            | \(3.6 \times 10^3\)            | 5.9                             | 5.9                             | 0.49                            |
| 25.0 (full)| \(2.3 \times 10^5\)           | \(1.8 \times 10^5\)            | \(5.0 \times 10^4\)            | 2.7                             | 2.7                             | 0.20                            |
| (sub-region)| \(5.8 \times 10^4\)           | \(3.8 \times 10^4\)            | \(2.0 \times 10^4\)            | 3.3                             | 3.3                             | 0.41                            |
| 33.7 (full)| \(2.7 \times 10^5\)           | \(1.7 \times 10^5\)            | \(1.1 \times 10^5\)            | 2.2                             | 2.2                             | 0.28                            |
| (sub-region)| \(8.0 \times 10^4\)           | \(3.2 \times 10^4\)            | \(4.7 \times 10^4\)            | 2.5                             | 2.5                             | 0.55                            |
will explore the possibility of doing so, taking advantage of our having the full information about the fluid variables available in our simulated volume.

Averaging all H\textsubscript{i} brightness profiles in the gridded cube leads to relatively featureless profiles (Figure 6, left column), although they do show that the velocity dispersion of the gas in the gridded cubes decreases as time progresses, due to the decaying turbulence. On the other hand, zooming into a specific region of the simulation box where molecular gas has formed yields profiles with more structure. Most notably, the profiles display the familiar central depression (Figure 6, right column).

Since the smaller region is selected to be approximately at the same spatial location at all three times shown, the averaged profile changes significantly from one time to the other. At the middle time, very little structure is present, while at the other timesteps more structure is seen, which is most likely caused by converging flows of gas. Finally, to show the qualitative agreement, we show in Figure 7 an averaged H\textsubscript{i} profile of the main Taurus region, using data from the Arecibo GALFA-H\textsubscript{i} (Peek et al. 2011) survey. Particularly, the velocity dispersion is comparable. The Taurus cloud is estimated to have linear dimensions of 32 × 5 pc (e.g., Ballesteros-Paredes et al. 2009). Our simulation volume is large enough to contain Taurus-like structures. The velocity dispersion at the earlier time shown from our simulation is the closest to what is seen in Taurus, consistent with the view that the Taurus area is still relatively young (e.g., Hartmann et al. 2001; Luhman et al. 2003, 2007; Pineda et al. 2010).

5 MOLECULAR GAS AND HISA

5.1 Identifying H\textsubscript{i} self-absorption features

In Heiner & Vázquez-Semadeni (2013), we used the second derivative of the H\textsubscript{i} profile as a tracer for H\textsubscript{i} self-absorption, and by extension, as a tracer for cold atomic gas. This approach was inspired by Krčo et al. (2008), who used the second derivative of the H\textsubscript{i} line profile in combination with molecular (CO) emission line data to correct the H\textsubscript{i} profiles for self-absorption. Their rationale was that H\textsubscript{i} line profiles are approximately gaussian in nature, and that the profiles of HISA are much narrower than those of the background emission, so that an H\textsubscript{i} self-absorption feature will become progressively more dominant in progressively higher derivative profiles, while the overall emission profile will fade into the background. Krčo et al. (2008) concluded that using the second derivative is sufficient to locate potential self-absorption features with relative ease. Additionally, they required the presence of CO emission: When it was present, they referred to this as ‘H\textsubscript{i} narrow self-absorption’, or HINSA for short, although we will stick to the more general term HISA here. In what follows, we will explore the uncertainties involved in using the second derivative of the H\textsubscript{i} profile, whether or not supplemented by CO observations.

In the top panel of Figure 8 we show typical H\textsubscript{i} line profiles, and their first and second derivatives respectively in the middle and bottom panels. The black lines represent a profile from our simulation at 12.5 Myr at an arbitrary location, whereas the gray line represents a typical H\textsubscript{i} profile from the Taurus molecular cloud, from the GALFA survey. It can indeed be seen that the dips in the profiles become prominent in the second derivative, since sharper dips produce stronger features in the second derivative. The Taurus profile is starting to be dominated by noise in the second derivative, but its HISA-indicating peak is still prominent.
Figure 6. Left column: Averaged brightness temperature profiles of the full gridded cubes are displayed with one-sigma deviations from the average value as dashed lines. It can be seen that the velocity dispersion is becoming lower at later times. Right column: The same averaged temperature profiles with one-sigma deviations are shown as in the previous figure, but for a specific region of the simulation box. More structure in the profiles can be seen in this case; in particular, dips.

Note that the wings of the second derivative of the profile in the synthetic case are much more prominent, which is a result of our brightness temperature profiles being steeper than a typical Taurus profile. This property is an important clue to the composition and physical conditions of the gas, but a more thorough investigation of this issue is beyond the immediate scope of this work.

As mentioned above, it is often unclear from observations of the $\text{HI}$ line profile whether a dip in the profile is caused by self-absorption or by a lack of atomic gas. Depending on the local morphology of the cloud, the lack of atomic gas may imply the presence of molecular gas, but then an additional tracer of the molecules is needed. Figure 9 shows, for the position on the $(y,z)$ plane used in Figure 8, the density, temperature, velocity distribution and visual extinction along the $x$ spatial coordinate, as well as the brightness temperature, its second derivative, opacity and atomic column density per velocity interval (in the velocity coordinate). Hennebelle et al. (2007) showed similar plots and noted that individual cloudlets cannot be distinguished observationally along the line of sight due to thermal broadening. The same can be seen in our figure.

Since our goal is to test how well HISA correlates with the molecular emission, we need to make sure that what we identify as HISA is indeed due to $\text{HI}$ self-absorption, and not just to a lack of emission. To this end, we take advantage of the fact that the radiative transfer code producing the $\text{HI}$ line profile also records the local opacity. Thus, we can easily search for those instances where dips in the $\text{HI}$ profile closely match peaks in the opacity ($\tau_v$) along the velocity coordinate.

Figure 10 illustrates this process for a profile with an emission dip matched by an opacity peak (left panel), a non-HISA profile (middle panel), and a slightly more complex profile (right panel) — all taken from individual positions in the simulation. The peak in the opacity does not have
Figure 9. Plots showing the profile from Figure 8 with various quantities to illustrate the structure behind the H\textsc{i} profile. The quantities shown are: Total gas density $\rho$, $T$, $v_x$, and $A_v$, as well as the H\textsc{i} brightness temperature and its second derivative, the opacity $\tau_x$ (plotted as the extinction $1 - \exp(-\tau_x)$) and the fractional $N_{\text{atom}}$.

to be exactly at the same velocity as the minimum brightness temperature of the H\textsc{i} profile dip, as there could be foreground or background material emitting in the same velocity interval, partially filling up the dip and displacing it from the opacity peak. We thus (arbitrarily) choose to find opacity peaks in a range of $\pm0.6$ km s$^{-1}$, or four velocity channels in each direction.

Not all instances of H\textsc{i}S A are located this way, though, as the profile on the right panel of Fig. 10 illustrates. The second opacity peak in this plot results in an inflexion point in the H\textsc{i} profile, which we do not count as H\textsc{i}S A, since we only flag local minima. But at least we guarantee that everything that we label as H\textsc{i}S A indeed corresponds to self-absorption. Additionally, we record the depth of the H\textsc{i}S A-induced feature relative to the adjacent peaks in the profile, a quantity we refer to as the dip depth. We use this information to check for correlations between the depth of the H\textsc{i}S A features and the local molecular gas content.

Applying this H\textsc{i}-minimum-opacity-peak matching process for every spatial pixel, we obtain a mask of locations where true H\textsc{i}S A is detected. We will refer to this as the H\textsc{i}S A mask map. In addition to being a mask, however, this map contains the values of the H\textsc{i}S A dip depth, thus providing not only an on/off switch for where ‘true H\textsc{i}S A’ is detected, but also a measure of the strength of the absorption feature. When we consider these values for comparison,
we will indistinctly refer to this as the ‘HISA dip depth map’. To reduce the number of false positives, we also require that the matching opacity peak be closer to the dip in $T_b$ than the nearest opacity (local) minimum. This mask can then be compared to the HISA derived from the second-derivative method and to molecular gas emission.

5.2 Strength of the HISA features compared to the ‘real’ HISA

Analogously to the procedure inspired by Krčo et al. (2008) that we used in Heiner & Vázquez-Semadeni (2013), we have constructed a ‘HISA strength’ map that is simply the maximum minus the minimum value of the second derivative of the H I brightness temperature profile ($T_{\text{max}} - T_{\text{min}}$). Since narrow self-absorption starts to feature prominently in the second derivative of the line profile, measuring the largest local difference in its value can be considered a reasonable proxy for the presence and the amplitude of the HISA feature. However, based on the H I profile alone one cannot distinguish between HISA and the lack of atomic gas, which is why Krčo et al. (2008) required the presence CO emission at the position on the plane of the sky (POS) where H I was to be identified, as a condition to declare the reduced H I emission as indicative of HISA. In Heiner & Vázquez-Semadeni (2013), we did not explicitly require CO emission, but the region of interest (Taurus) is a well-known molecular cloud, with a well-known presence of CO, so dropping the CO requirement had no obvious consequences. Now, we can begin to use our simulation to estimate how reliably the HISA strength map, by itself, traces HISA.

Figure 11 shows, from left to right, the HISA strength map, the HISA mask and the integrated CO intensity. It can be seen that the HISA strength map shows the most features, which in part can be seen on the HISA mask. Finally, only a small fraction of the features in either map are seen in CO emission.

By using the term HISA strength, we assume (or imply) that higher values of HISA strength correspond to higher odds of a particular pixel in the map representing actual HISA. In reality, there is no clear relation between the HISA strength and any actual HISA amplitude. Still, we test this assumption in Figure 12 by showing how well the pixels in the HISA strength map correspond with the HISA mask.

In order to make this comparison, we adopted a slightly different definition of HISA strength that allows different thresholding values, namely, we used increasing threshold values of the integrated second derivative of the H I profile, summing the contributions of the points along the LOS that are above the threshold. This allows us to consider a scale of increasing HISA strength. As this threshold is increased, fewer and fewer pixels will be captured in the spatial plane. Thus, we only count the number of pixels that are left after applying each threshold value, and then check how many of those pixels also lie on the HISA mask.

We define a ‘match success rate’ as the percentage of pixels where the HISA strength pixels above a certain threshold match with corresponding HISA mask pixels (implicitly assuming the HISA mask to be superior, although not perfect). We also counted the percentage of pixels in the HISA mask map that are above the threshold in the HISA strength map. This latter percentage drops monotonically with increasing values of the threshold, the number of points with which this is achieved goes down. For lack of a perfect correspondence, a balance should be achieved between the success rate and the number of pixels with which this is achieved goes down. For lack of a perfect correspondence, a balance should be achieved between the success rate and the number of pixels with which this is achieved if one were to optimize the detection of HISA.

Since we already noted that the HISA strength map and the HISA mask agree well on a coarse scale, but less accurately on a fine scale (cf. Fig. 11), we also check for nearby HISA mask pixels for every HISA strength map pixel, which is effectively a form of smoothing. Figure 12 also shows the success rates when HISA mask pixels are found within one, two and three pixels respectively, where by ‘a distance of one pixel’ we mean that we search within a $3 \times 3$-pixel box (or, equivalently, in a $1.5 \times 1.5$-pc box) with the HISA strength map pixel at the center. Interestingly, even searching within just one pixel already doubles the typical success rate, while searching within three pixels (a $3.5 \times 3.5$-pc box) approximately quadruples the original success rate or more. This means that, while the HISA strength maps do not corre-
Figure 11. Left column: HISA strength maps at the three timesteps we study (with time increasing from top to bottom), where the HISA strength is defined as the maximum difference between values of the second derivative of the brightness temperature profile as in Heiner & Vázquez-Semadeni (2013). Middle column: the HISA mask, or ‘real HISA’, defined as the set of pixels in a projection of the simulation where local minima in the $\text{H}_i$ line profile coincide with peaks in the optical depth. While the major cloud structures are visible in both the left and middle columns, the correspondence is far from perfect. Right column: Integrated CO intensity maps are shown for the two timesteps where CO emission is present.

Comparing the three different timesteps, the first thing to note is the sharp drop in the percentage reflecting the number of pixels above the threshold values. At the highest threshold value, this percentage reaches a nearly zero value in all three timesteps, indicating that applying a higher threshold will yield no improvement. Next, for the first timestep we see that the success rate increases sharply with an increasing threshold, although the number of pixels in the mask drops sharply as well. However, for the other two timesteps the success rate does not rise as sharply with an increasing threshold, even when smoothing is applied. Basically, in these cases, increasing the threshold value does not significantly improve the correspondence, and the only way to improve it is to apply smoothing.

One potential problem with using the second derivative of the brightness temperature profile ($\Delta T_b$) is that in our simulations, the wings of the profile become very prominent in the $\Delta T_b$ profile, which is indicative of steep line profile wings (see e.g. Figure 8). In the $\Delta T_b$ profile, these wings can have higher amplitudes than the peak caused by HISA at the center of the profile. Because of our definitions of HISA strength that are directly related to the amplitude of $\Delta T_b$, it is possible that our HISA strength measures are contaminated by $\Delta T_b$ profiles that are purely steep with no absorption feature. By comparison, the Taurus line profiles have relatively broad and shallow wings and therefore do not suffer from this problem: the peak in $\Delta T_b$ is caused almost exclusively due to dips in the center of the $T_b$ profile. However,
Figure 12. ‘Match success rate’, or fraction of pixels in the HISA strength map (left column of Fig. 11) above a certain threshold value that coincide with the HISA mask (middle column of Fig. 11), shown percentage-wise, as a function of the threshold value, for the three timesteps studied (solid line with circular dots). The dashed grey lines with upright triangles, squares, pentagons and hexagons represent the match success rate with pixels within distances of 1, 2, 3, and 4 pixels, respectively. The solid line with upside-down triangular markers shows the number of pixels above the threshold value as a percentage of the number of pixels in the HISA mask.

Figure 13. The same quantities are plotted as in Figure 12 but calculated from a HISA strength map with the wings on both ends of $T''_b$ blanked out. No significant improvement in the success rate was obtained by applying the wing blanketing.

this could be due partially to the poorer velocity resolution of the Taurus data.

In order to see whether this contamination influenced our success rate, we blindly blanketed out (i.e. set $T''_b$ to 0) the outer wings of the second derivative. This is fairly trivial since all emission profiles increase initially from both ends of...
the velocity axis towards a peak. The resulting success rate plots are shown in Figure 13, where it can be seen that this procedure has very little if any effect on the success rate. In other words, the steep profiles and the resulting dominant wings in the second derivative of the line profile do not cause significant problems in the identification of HISA features.

5.3 Comparing HISA to the CO emission

After considering to what extent HISA strength maps can trace actual HISA, we will now look at the connection between HISA and molecular gas: Firstly, the CO gas. A one-to-one relation should not be expected, since HISA itself is caused by atomic rather than molecular gas, but it is generally thought that the presence of HISA is a sign of atomic gas in the process of turning molecular. Therefore, HISA should at least be expected to occur near molecular gas.

In the top panels of Figure 14 we show qualitatively how the atomic gas ($N_{\text{HI}}$, grayscale) and the CO emission ($W_{\text{CO}}$, thin red contours) relate to the HISA mask map (thick blue contours). We remind the reader that no CO emission was produced at the first timestep. In the bottom panels of Figure 14 we zoom into a smaller region (roughly the same region in all three timesteps). It can be seen that the HISA mask dip depth contours mostly border the CO emission contours as one might expect from cold atomic gas moving towards sites where it turns molecular.

We compared the two HISA measures to the integrated CO emission and found a very poor correlation (if any), even after averaging the data to $8 \times 8$-pc pixels, as shown in Figure 15. The averaging size was chosen based on the possible projected position in the POS.

### Table 2

| Time (Myr) | Res. (pc) | $r_{\text{strength}}$ | $r_{\text{match}}$ |
|------------|----------|-----------------------|-------------------|
| 12.5       | 1        | 0.38                  | 0.19              |
| 2          |          | 0.44                  | 0.26              |
| 4          |          | 0.53                  | 0.35              |
| 8          |          | 0.65                  | 0.55              |
| 16         |          | 0.75                  | 0.79              |
| 25.0       | 1        | 0.33                  | 0.20              |
| 2          |          | 0.40                  | 0.26              |
| 4          |          | 0.48                  | 0.33              |
| 8          |          | 0.56                  | 0.50              |
| 16         |          | 0.64                  | 0.59              |
| 33.7       | 1        | 0.26                  | 0.17              |
| 2          |          | 0.33                  | 0.25              |
| 4          |          | 0.42                  | 0.42              |
| 8          |          | 0.50                  | 0.61              |
| 16         |          | 0.54                  | 0.72              |

Table 2. Pearson $r$ correlation values as a function of increasing pixel size for the HISA strength ($r_{\text{strength}}$) and HISA mask map ($r_{\text{mask}}$).

though the HISA strength and HISA mask maps are not identical.

### Table 2

| Time (Myr) | Res. (pc) | $r_{\text{strength}}$ | $r_{\text{match}}$ |
|------------|----------|-----------------------|-------------------|
| 12.5       | 1        | 0.38                  | 0.19              |
| 2          |          | 0.44                  | 0.26              |
| 4          |          | 0.53                  | 0.35              |
| 8          |          | 0.65                  | 0.55              |
| 16         |          | 0.75                  | 0.79              |
| 25.0       | 1        | 0.33                  | 0.20              |
| 2          |          | 0.40                  | 0.26              |
| 4          |          | 0.48                  | 0.33              |
| 8          |          | 0.56                  | 0.50              |
| 16         |          | 0.64                  | 0.59              |
| 33.7       | 1        | 0.26                  | 0.17              |
| 2          |          | 0.33                  | 0.25              |
| 4          |          | 0.42                  | 0.42              |
| 8          |          | 0.50                  | 0.61              |
| 16         |          | 0.54                  | 0.72              |

Table 2. Pearson $r$ correlation values as a function of increasing pixel size for the HISA strength ($r_{\text{strength}}$) and HISA mask map ($r_{\text{mask}}$).

Comparison to the CO emission

In order to show the distribution of the gas density in the simulation volume, we produced the (volume weighted) vol-

### 6 GENERAL STRUCTURE OF THE CLOUDS

#### 6.1 Evolution of the PDFs

In order to show the distribution of the gas density in the simulation volume, we produced the (volume weighted) vol-
Figure 14. The spatial distribution of the atomic hydrogen column density (grayscale), the integrated CO intensity (thin red) and the depth of the dip caused by HISA (thick blue) are displayed for each timestep (top panels). We used one HISA mask contour of 5 K and three \( W_{\text{CO}} \) contours of 0.1, 1 and 10 K km s\(^{-1}\). The bottom panels show a zoomed-in section of the top panels. These sections are marked with white rectangles in the top panels. A color version of this figure is available in the online version of this journal.

Figure 15. Integrated CO emission \( W_{\text{CO}} \) against the HISA strength (original definition as used in Heiner & Vázquez-Semadeni (2013), left panel) and HISA mask dip depth (right panel) using a pixel size of 8 pc\(^2\).

We note that all \( \rho \)- and column (\( N \)) density probability density functions, as plotted in Figures 18 and 19. In all cases we fit (by-eye) a log-normal gaussian to the higher density end of the distribution to draw attention to the qualitative shape of the PDFs.

The log-normal shape of the \( \rho \)-PDFs is expected to occur for nearly isothermal flows when no star formation is happening and the flow is turbulence-dominated. In our case this is particularly obvious in the first timestep, when molecular gas already exists but is not enough to result in CO emission. Conversely, in the two last timesteps, when gravity has become the dominant driving force, a power-law tail is seen to have developed at the high density end of the
PDFs (Figure 18 first and third columns). This is caused by the molecular gas part of the gas, as can be seen in the third column of Figure 18 whereas the PDFs in Figure 19 (depicting the atomic gas) show no obvious power-law tails. It should also be noted that the power-law tail in the molecular column density PDFs (Figure 18 right two columns) is not so prominent due to line-of-sight confusion. Although not a conclusive proof, these results are consistent with, and strongly support, the scenario that molecules themselves are not necessary for gravitational collapse, and that instead they are formed as a consequence of collapse in all three directions allowing a visual extinction above unity to be achieved (Hartmann et al. 2001; Heitsch & Hartmann 2008; Glover & Clark 2012).

Figure 19 also shows both the atomic gas N-PDF (computed directly from the simulation; middle column) and the...
column density PDF ($N_{\text{HI}}$-PDF) derived from the synthetic observations (right column). It can be seen that the column densities derived from the synthetic observations have a smaller dynamic range: The gas column becomes optically thick at a value of several times $10^{21}$ cm$^{-2}$, which in turn causes HI self-absorption features to appear in the line profiles. Conversely, the atomic column density shows a larger dynamic range since it is computed directly from the simulation before the effects of self-absorption are taken into account. The column density values are limited because the gas ultimately becomes molecular. Otherwise the profiles look qualitatively the same: a low-density background-level peak and a log-normal shape.

### 6.2 Accretion onto molecular clouds and kinematics

As discussed in Sec. 5, the dense molecular clouds in the simulation grow by accretion of HI gas. It is thus important to investigate the signatures of this process in the observational domain. Figure 20 shows the HI and CO brightness temperature (contours and grayscale respectively) at the last two timesteps (top and bottom rows, respectively), and in two velocity intervals, from $-15$ to $0$ km s$^{-1}$ and from $0$ to $+15$ km s$^{-1}$ (left and right columns, respectively). Different subregions of the simulation were chosen in each timestep, so that each was centered on a prominent cloud structure at the given timestep. The first timestep ($t = 12.5$ Myr), is not shown because, as mentioned above, no CO emission is produced at that time.

There is only a very vague structure visible of CO gas surrounded by atomic gas, possibly due to projection effects. We also note that channel maps such as these may show more small-scale structure than the three-dimensional maps, or slices through these maps. The reason for this is that there is no strictly uniform relation between the velocity and the spatial axis, a certain amount of randomization of the structure takes place (Pichardo et al., 2000).
Figure 18. Volume- and column-density PDFs at all three timesteps studied in the simulation. The left panels show the total gas PDFs, whereas the right panels show the molecular gas PDFs. By-eye fits of the gaussian component of each PDF are shown with dashed lines to draw attention to the qualitative structure of the PDFs.

Figure 19. Volume density PDFs of the atomic gas (left column), and column density PDFs of the atomic gas, either derived directly from the simulation \(N_{\text{atom}}\) (middle column) or derived from the synthetic H\(_i\) line profiles \(N_{\text{HI}}\) (right column). By-eye fits of the log-normal component of each PDF are shown by the dashed lines.

In Figure 21 we plot cuts of the density field of both the H\(_i\) (thin black contours) and the molecular (thick purple contours) gas density on the \((x,z)\)-plane, as well as the projection of the velocity vector on this plane (grey arrows) and the \(x\)-component of the velocity field (color scale). The green colors indicate a positive velocity, from left to right along the x-axis, whereas the brown colors indicate the opposite direction. In the middle and right panels of Figure 21 we show the line profiles extracted from the same regions, as seen by an observer at the right of the fields (middle panels) or from above them (right panels). It is clear from these figures that the H\(_i\) gas is in the process of accreting onto the dense molecular cloud.

The top-left panel of Figure 21 (at \(t = 12.5\) Myr) shows that the dense structure on the left side of the field, centered at \((x,z) \approx (25,100)\) pc, and which contains both H\(_i\)
Synthetic observations H\textit{i} and molecular gas

Figure 20. Thick slices in velocity space (-15 to 0 and 0 to 15 km/s) of the H\textit{i} and CO brightness temperatures are shown in contours and grayscale respectively, integrated to $N_{\text{HI}}$ and $W_{\text{CO}}$ respectively. The H\textit{i} contours are 4, 6, 8, 10, 12 and $14 \times 10^{20}$ cm$^{-2}$, with the lowest contour level colored gray. Only the two later timesteps are shown since no CO emission was present in the first timestep.

and (CO-free) molecular gas, is accreting diffuse H\textit{i} material predominantly along the vertical ($z$) direction. There is also a converging flow along the $x$-direction, with the collision region centered roughly at ($x, z$) $\approx$ (90, 90) pc, but this flow seems to not have formed a dense cloud yet, and instead it seems to be carrying previously formed, predominantly atomic clouds spanning the ranges ($\Delta x, \Delta z$) $\approx$ (50:80, 80:90) pc and ($\Delta x, \Delta z$) $\approx$ (110:130, 80:110) pc, respectively. In the middle-left panel ($t = 25$ Myr), the flow seems to have joined the two components described above into a single, long filament stretching along most of the $x$-extension of the region, with the positive (blue) and negative (brown) components of the $x$ velocity being located below-left and above-right of the cloud complex, respectively. The complex is highly molecular at the left, but still mostly atomic at the right part of the field. Finally, in the bottom-left panel, the complex is seen to have become mostly molecular, and is still accreting diffuse H\textit{i} material mostly along the vertical ($z$)-direction. Although not shown here, at this time the cloud is copiously forming stars.

In the middle and right panels, we note that the accretion process often results in double-peaked H\textit{i} line profiles. Such features are common in observations of H\textit{i} in the neighborhood of molecular clouds (see, e.g., the top panel of Fig. 8), and our results from this Section suggest that such bimodal profiles are often the result of the H\textit{i} flow onto the molecular clouds.

7 DISCUSSION AND CONCLUSIONS

7.1 Limitations

One of the key missing features in the present study is the inclusion of supernova (SN) feedback, which should maintain the turbulence driving at the scales of our simulation. This may, in turn, have a significant effect on the evolution and structure of the clouds, although its relative importance compared to the gravitational driving of the motions in the clouds is uncertain. Supernovae tend to explode in regions that have been previously evacuated by ionizing radiation and winds from the massive stars, and numerical simulations of this scenario (albeit without self-gravity) suggest that the dense clouds are not strongly affected by the supernovae (e.g., de Avillez & Breitschwerdt 2004 Hill et al. 2012). In a future study, we plan to repeat our analysis in...
the presence of ionization and SN feedback, as well as the magnetic field and ambipolar diffusion.

Another important and obvious improvement we can make to our model is a more detailed treatment of the formation and destruction of molecular gas (cf. e.g. Smith et al. 2014). For example, we assume that the formation of molecular gas happens on a timescale that is very small relative to the timesteps we considered, but if we follow the evolution of the gas particles more closely a minimum timescale for molecular gas formation can be imposed as well as a certain balance of photodissociation. As a consequence, the molecular and CO fractions in our simulation must be considered as upper limits. At least our approach provides a first order approximation to the evolution of atomic and molecular gas.

7.2 Summary

We have presented a numerical simulation where ‘molecular’ clouds are identified by using a post-facto processing of the particles in the simulation volume: molecular gas was assumed to have formed if the local temperature had dropped below 50 K and the local average extinction, \( A_v > 1 \). We also created synthetic observations of Hi and CO, the latter assumed to exist at a grid cell if the conditions for molecular gas were satisfied and besides the local density satisfied \( n > n_{\text{crit}} \), where \( n_{\text{crit}} \) is the critical density for CO formation (cf. Sec. 2.2).

We used two different methods to identify (potential) HISA features. One, we used the amplitude of the second derivative of the H I brightness temperature profile, dubbed ‘HISA strength’. Two, we identified HISA features by matching local minima in the H I brightness temperature profile to peaks in the calculated opacity at the same velocity (that we call ‘HISA mask’), thereby distinguishing between dips in the profile caused by H I and those caused by the absence of atomic gas. Although this method is superior because it uses local gas opacity information, it cannot be applied to actual observations since this kind of information is generally not available. Nevertheless, it provides a means of testing the goodness of the first method. We then compared the location and intensity of the H I features with the presence of molecular gas and looked at the structure of the gas. Finally, we investigated the density and column-density PDFs of the gas, the latter obtained both directly from the simulation data and from the synthetic observations. We focused on three timesteps of the simulation, namely at \( t = 12.5, 25 \) and 33.7 Myr. The first timestep corresponds to a time when the clouds are still developing and no SF is occurring in the simulation. The second corresponds to a time when SF is at an early phase, while the latter corresponds to a time when SF is copious. At this time, the effects of stellar feedback are clearly missing and should be included in future studies. Our main results were as follows:

- At the first of the timesteps studied, significant quantities of molecular gas exist, but no significant CO has formed yet. That is, the molecular gas is ‘CO-free’. Instead, at the last of the three timesteps, CO is abundant. This result is consistent with the scenario that gravitational contraction drives the formation of CO molecules (cf. Heitsch & Hartmann 2008).
- At the chosen resolution of our gridded data (0.5 pc pixel separation), there is a very poor spatial correlation between the H I strength and the H I mask. The correlation improves if matches with neighbouring pixels (in the projected plane of the sky, POS) are allowed.
- However, both H I NSA indicators show a weak but signif-

Figure 21. Left panels: Slices of the atomic (thin black contours) and molecular (thick purple contours) gas density on the \((x,z)\)-plane in a subregion of the simulation containing an evolving massive cloud, shown at the three timesteps investigated throughout the paper. The arrows show the projection of the velocity vector on this plane, and the color scale depicts the value of the \(x\)-component of the velocity on the plane. A positive value of this component means a flow from left to right in the figure. A color version of this figure is available in the online version of this journal. In the middle and right panels, we show the H I brightness temperature profiles resulting from these regions, as observed from the positive-\(x\) direction (middle panels) and from the positive \(z\) direction (right panels). It is seen that the peaks of the H I emission correspond to the typical values of the H I velocity approaching the molecular gas. As before, the dashed lines mark 1-\(\sigma\) deviations from the average line profile. Note that the profiles in the \(z\)-direction are less pronounced because they span the full \(z\)-coordinate range, but the selected gas structures as shown in the left panels only span a small fraction of the \(z\)-coordinate range.
icant correlation with the molecular gas column density on a scale of a few to several parsecs on the POS. At smaller scales no correlation is visible. This suggests that HISA is located on the periphery of the molecular emission, rather than coincident with it.

• The volume and column density PDFs extracted from the simulation show the expected transition from a purely log-normal shape to one with a power-law tail when molecular clouds form. However, the power-law tail is only seen in the molecular components, and not in the HI, suggesting that molecule formation is directly correlated with gravitational infall.

• At least in our simulation, most of the multi-peaked HI line profiles in the neighborhood of molecular clouds are caused by bulk HI flows into the molecular clouds, rather than by HI self-absorption.

ACKNOWLEDGMENTS

JSH and the computer cluster on which the numerical simulations were carried out are supported by CONACYT grant 102488 to Enrique Vázquez-Semadeni.

REFERENCES

Audit E., Hennebelle P., 2005, A&A, 433, 1
Ballesteros-Paredes J., D’Alessio P., Hartmann L., 2012, MNRAS, 427, 2562
Ballesteros-Paredes J., Gómez G. C., Loinard L., Torres R. M., Pichardo B., 2009, MNRAS, 395, L81
Ballesteros-Paredes J., Hartmann L., 2007, Revista Mexicana de Astronomía y Astrofísica, 43, 123
Ballesteros-Paredes J., Hartmann L., Vázquez-Semadeni E., 1999, ApJ, 527, 285
Ballesteros-Paredes J., Mac Low M.-M., 2002, ApJ, 570, 734
Banerjee R., Horn S., Klessen R. S., 2009a, in Protostellar Jets in Context, Tsinganos K., Ray T., Stute M., eds., Springer, Berlin, pp. 421–427
Banerjee R., Vázquez-Semadeni E., Hennebelle P., Klessen R. S., 2009b, MNRAS, 398, 1082
Blitz L., 1993, in Protostars and Planets III, Levy E. H., Lunine J. I., eds., pp. 125–161
Cernicharo J., Bachiller R., 1984, A&AS, 58, 327
Clark P. C., Glover S. C. O., 2013, ArXiv e-prints
Clark P. C., Glover S. C. O., Klessen R. S., Bonnell I. A., 2012, MNRAS, 424, 2599
Colín P., Vázquez-Semadeni E., Gómez G. C., 2013, MNRAS de Avillez M. A., Breitschwerdt D., 2004, A&A, 425, 899
Dobbs C. L., Pringle J. E., Naylor T., 2014, MNRAS, 437, L31
Draper P. W., Currie M. J., Jenness T., Leech J., Economou F., Berry D. S., Taylor M. B., 2007, in Astronomical Society of the Pacific Conference Series, Vol. 376, Astronomical Data Analysis Software and Systems XVI, Shaw R. A., Hill F., Bell D. J., eds., p. 695
Elmegreen B. G., Scalo J., 2004, AR&AA, 42, 211
Franco J., Cox D. P., 1986, Publications of the Astronomical Society of the Pacific, 98, 1076
Gazol A., 2013, ApJ, 765, 49
Gazol A., Vázquez-Semadeni E., Kim J., 2005, ApJ, 630, 911
Gibson S. J., Taylor A. R., Higgs L. A., Brunt C. M., Dewdney P. E., 2005, ApJ, 626, 214
Gibson S. J., Taylor A. R., Higgs L. A., Dewdney P. E., 2000, ApJ, 540, 851
Glover S. C. O., Clark P. C., 2012, MNRAS, 421, 9
Goldsmith P. F., 2005, ApJ, 622, 938
Gomez G. C., Vázquez-Semadeni E., 2013, ArXiv e-prints
Hartmann L., Ballesteros-Paredes J., Bergin E. A., 2001, ApJ, 562, 852
Heiner J. S., Vázquez-Semadeni E., 2013, MNRAS, 429, 3584
Heitsch F., Ballesteros-Paredes J., Hartmann L., 2009, ApJ, 704, 1735
Heitsch F., Hartmann L., 2008, ApJ, 689, 290
Hennebelle P., Audit E., Miville-Deschênes M.-A., 2007, A&A, 465, 445
Hennebelle P., Banerjee R., Vázquez-Semadeni E., Klessen R. S., Audit E., 2008, A&A, 486, L43
Hill A. S., Joung M. R., Mac Low M.-M., Benjamin R. A., Haffner L. M., Klingenberg C., Waagan K., 2012, ApJ, 750, 104
Jappsen A.-K., Klessen R. S., Larson R. B., Li Y., Mac Low M.-M., 2005, A&A, 435, 611
Kavars D. W., Dickey J. M., McClure-Griffiths N. M., Gaensler B. M., Green A. J., 2005, ApJ, 626, 887
Knapp G. R., 1974, AJ, 79, 527
Koyama H., Inutsuka S.-I., 2000, ApJ, 532, 980
Krče M., Goldsmith P. F., 2010, ApJ, 724, 1402
Krče M., Goldsmith P. F., Brown R. L., Li D., 2008, ApJ, 689, 276
Li D., Goldsmith P. F., 2003, ApJ, 585, 823
Luhman K. L., Allers K. N., Jaffe D. T., Cushion M. C., Williams K. A., Shesnick C. L., Vacca W. D., 2007, ApJ, 659, 1629
Luhman K. L., Briceño C., Stauffer J. R., Hartmann L., Barrado y Navascués D., Caldwell N., 2003, ApJ, 590, 348
Mac Low M.-M., Klessen R. S., 2004, Reviews of Modern Physics, 76, 125
Molinari S. et al., 2014, ArXiv e-prints
Ostriker E. C., Stone J. M., Gammie C. F., 2001, ApJ, 546, 980
Peek J. E. G. et al., 2011, ApJS, 194, 20
Pichardo B., Vázquez-Semadeni E., Gazol A., Passot T., Ballesteros-Paredes J., 2000, ApJ, 532, 353
Pineda J. E., Caselli P., Goodman A. A., 2008, ApJ, 679, 481
Pineda J. L., Goldsmith P. F., Chapman N., Snell R. L., Li D., Cambrésy L., Brunt C., 2010, ApJ, 721, 686
Rohlfs K., Wilson T., 1996, Tools of Radio Astronomy, 2nd ed. Springer, Berlin, New York
Smith R. J., Glover S. C. O., Clark P. C., Klessen R. S., Springel V., 2014, ArXiv e-prints
Springel V., Yoshida N., White S. D. M., 2001, New Astron., 6, 79
Vázquez-Semadeni E., Banerjee R., Gómez G. C., Hennebelle P., Duffin D., Klessen R. S., 2011, MNRAS, 414, 2511

© 201X RAS, MNRAS
Vázquez-Semadeni E., Colín P., Gómez G. C., Ballesteros-Paredes J., Watson A. W., 2010, ApJ, 715, 1302
Vázquez-Semadeni E., Gazol A., Scalo J., 2000, ApJ, 540, 271
Vázquez-Semadeni E., Gómez G. C., Jappsen A. K., Ballesteros-Paredes J., González R. F., Klessen R. S., 2007, ApJ, 657, 870
Vázquez-Semadeni E., Gómez G. C., Jappsen A.-K., Ballesteros-Paredes J., Klessen R. S., 2009, ApJ, 707, 1023