Turbulent mixing in the interstellar medium: an application for Lagrangian tracer particles

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Abstract

We use three-dimensional numerical simulations of self-gravitating compressible turbulent gas in combination with Lagrangian tracer particles to investigate the mixing process of molecular hydrogen (H\textsubscript{2}) in interstellar clouds. Tracer particles are used to represent shock-compressed dense gas, which is associated with H\textsubscript{2}. We deposit tracer particles in regions of density contrast in excess of 10\textsuperscript{ρ_0}, where \( ρ_0 \) denotes the mean density. Following their trajectories and using probability distribution functions, we find an upper limit for the mixing timescale of H\textsubscript{2}, which is of the order of 0.3 Myr. This is significantly smaller than the lifetime of molecular clouds, which demonstrates the importance of the turbulent mixing of H\textsubscript{2} as a preliminary stage to star formation.

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1. Introduction

Turbulent mixing of chemical species in the interstellar medium (ISM) has profound consequences on the morphology, chemistry, cooling and shielding of molecular clouds (MCs). MCs are known to be the formation site of young stars. It is a prerequisite for a successful theory of star formation to explain the physical and chemical environment in which stars are born. Measured velocity dispersions suggest that interstellar clouds exhibit internal supersonic compressible random motions, which are associated with turbulence (e.g. Larson 1981, Heyer and Brunt 2004). Kinetic energy power spectra in MCs have been measured (e.g. Padoan et al 2006), which are steeper than the Kolmogorov (1941) spectrum \( E(k) \propto k^{-5/3} \) of incompressible turbulence, even if intermittency corrections are considered (e.g. Boldyrev 2002, Kolmogorov 1962, Scheffe and Leveque 1994). High-resolution numerical simulations of supersonic compressible turbulence also yield velocity Fourier spectra closer to Burgers turbulence with typical values of \( E(k) \propto k^{-1.9} \) (e.g. Kritsuk et al 2007). Excellent summaries of empirical and theoretical aspects of interstellar turbulence are presented in the review articles by Elmegreen and Scalo (2004), Scalo and Elmegreen (2004) and Mac Low and Klessen (2004).

Compressions created by the formation of strong shocks facilitate the formation of molecular hydrogen, H\textsubscript{2} (e.g. Hollenbach et al 1971). Observations of MCs typically detect carbon monoxide as a tracer for H\textsubscript{2}, which is found to be ubiquitous throughout MCs and not merely in regions of high density. Turbulent transport of H\textsubscript{2} from high density to low density gas may be an explanation for its relative homogeneity.

A recent numerical investigation of interstellar turbulence by Glover and Mac Low (2007) confirms that turbulent compressions are a key mechanism for the rapid (1–2 Myr) formation of H\textsubscript{2}. Their results further suggest that a significant fraction of H\textsubscript{2} is located in low-density gas, in quantities greater than can be formed directly in situ. The authors propose that H\textsubscript{2} forms in shock-compressed sheets and filaments created by supersonic turbulence, and is subsequently transported to lower density regions. In order to test this hypothesis, we have performed simulations of interstellar turbulence that employ Lagrangian tracer particles...
to directly follow the trajectories of dense gas parcels. Tracer particles are deposited in high-density regions, formed in a driven compressible turbulent medium. We use statistical analysis to show that even under self-gravitating conditions, significant mixing of H$_2$ occurs on short timescales (<0.3 Myr).

In section 2, we describe our numerical scheme, tracer particles, turbulence forcing and simulation setup. Section 3 presents our results based on probability density functions, and in section 4, our conclusions are summarized.

2. Numerical methods and simulation setup

We solve the equations of compressible hydrodynamics including self-gravity on a three-dimensional static grid of 256$^3$ zones using the piecewise parabolic method (PPM) (Colella and Woodward 1984), implemented in the astrophysical code ENZO (O’Shea et al 2004) with periodic boundary conditions. Density $\rho$, velocity $v$, total energy density $\rho e$, pressure $P$ and gravitational potential $\Phi$ are related through the equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0,$$

(1)

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\frac{1}{\rho} \frac{\partial P}{\partial x} - \nabla \Phi + \mathbf{f},$$

(2)

$$\frac{\partial (\rho e)}{\partial t} + \nabla \cdot [v (\rho e + P)] = -\rho v \cdot (\nabla \Phi) + \rho v \cdot \mathbf{f},$$

(3)

$$\Delta \Phi = 4\pi G \rho,$$

(4)

where $G$ is the gravitational constant. An isothermal equation of state,

$$P = \rho (\gamma - 1) u \quad \text{with} \quad u = c - \frac{1}{2} v^2,$$

(5)

is approximated by $\gamma = 1.01$ is used to close the equations of hydrodynamics. This is a crude, but reasonable approximation on a wide range of scales in both length and density in interstellar clouds.

We start from a uniform distribution of gas, initially at rest. In order to excite turbulent motions, we utilize a stochastic forcing term $\mathbf{f}$, appearing as the source term in equations (2) and (3) that supplies kinetic energy on the largest scales. The forcing term has a parabolic Fourier spectrum with $k/k_0 = [0.5, 1.5]$ centered on $k_0 = 2\pi / L$, where $L$ is half of the size of the computational domain, and is evolved by an Ornstein–Uhlenbeck process (e.g. Esparain and Pope 1988, Schmidt et al 2006). In the present study, we adjust our forcing amplitude such that the fluid reaches a representative rms Mach number of 3. We emphasize that our forcing is constructed such that we can regulate the relative strength of compressive modes ($\nabla \times \mathbf{f} = 0$) with respect to solenoidal modes ($\nabla \cdot \mathbf{f} = 0$). The ratio of kinetic energies at the injection scale,

$$\chi = \frac{E_{\text{sol}}}{E_{\text{sol}} + E_{\text{comp}}},$$

(6)

is approximately 0.8 from solenoidal forcing. Note that $\chi$ is not exactly 1, because supersonic motions are excited at the injection scale, which always have compressive modes. For purely compressive forcing, we expect $\chi$ close to zero. This case will be investigated in a forthcoming paper.

Timescales are measured in units of the auto correlation timescale $T$ of the forcing, which was set equal to the turbulent crossing time on large scales for a Mach number 3 turbulent medium. This means that after approximately $1T$, the gas reaches an rms Mach number $M \approx 3$, which is maintained by the forcing for all times $t \geq 1T$. Within $0 \leq t < 1T$, self-gravity is kept deactivated, allowing the gas to reach a state of fully developed compressible turbulence. After that, at $t = 1T$, Lagrangian tracer particles are placed at the centers of grid cells with density $\rho / \rho_0 \geq 10$ ($\rho_0$ is the mean density), representing highly compressed gas parcels. From this point on, we distinguish three routes of further evolving the simulation:

1. no changes, self-gravity still deactivated (pure forcing);
2. self-gravity activated, representing 64 Jeans masses (forcing + SG4); and
3. self-gravity activated, representing 4096 Jeans masses (forcing + SG64).

Case 1 (pure forcing) serves as a control run to compare with the self-gravitating cases 2 and 3. The difference between 2 (SG4) and 3 (SG64) lies in the mean density $\rho_0$ of the fluid, which makes up a domain that contains a total of 64 Jeans masses for case 2 (SG4) and a total of 4096 Jeans masses for case 3 (SG64). We use the cubic definition of the Jeans mass

$$M_j = \rho_0 \lambda_j^3 = \rho_0 \left( \frac{\pi c_s^2}{G \rho_0} \right)^{3/2},$$

(7)

where $c_s = \sqrt{\gamma P / \rho}$ is the sound speed. Consequently, both self-gravitating cases have $M / M_j > 1$, where $M$ is the total mass in the domain. This represents gravitational...
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Figure 2. Temporal evolution of the spatial distribution of Lagrangian tracer particles (from top to bottom). Left: simulation without self-gravity (pure forcing). Right: simulation including self-gravity (forcing + SG64). Self-gravity can prevent some of the tracer particles from mixing with the background gas. There are no snapshots for $t > 1.2T$ for case SG64, because SG64 violates the resolution criterion for simulations including self-gravity (Truelove et al 1997) shortly after $t = 1.2T$, which only allows us to draw reliable conclusions up to this time. Case SG4 (not shown here) is statistically similar to the case of pure forcing, as discussed in the text.

unstable gas, and both cases would be subject to gravitational collapse in the absence of turbulent fluctuations and stochastic forcing.

The Langrangian tracer particles are evolved every time step (using a simple Euler-step) according to the Eulerian velocity, which is interpolated from the grid by means of a second-order accurate (triangular-shaped cloud) method at the current position of each tracer particle. We have also tried a first order (cloud in cell) and a third-order (tricubic; Lekien and Marsden 2005) spatial interpolation, and a predictor–corrector-step for time integration, which yielded no statistically significant differences.
Figure 3. Time sequence of the mass-weighted density PDFs for the case without self-gravity (pure forcing). The Lagrangian PDF of the tracer particles (solid line) gradually approaches the Eulerian PDF (dashed line). The last frame represents a much later time \( t \approx 3T \), which shows that apart from statistical fluctuations, the PDFs do not change significantly anymore for \( t \gtrsim 1.3T \). Dotted lines are least-squares fits using the log-normal distribution given by equation (8).

3. Results and discussion

Figure 1 shows the spatial distribution of tracer particles at \( t = 1.0T \), the instant of their deposition, which serves as an initial condition for three different routes of further development (see section 2). Approximately 24,000 tracer particles have been placed in regions of shock-compressed gas with density contrast in excess of 10, representing H\(_2\) in the following. In figure 2, we compare the evolution of the pure forcing run (left panel) to the ‘strong’ self-gravitating case SG64 (right panel). The case of ‘weak’ self-gravity (SG4) is not shown here, because it is almost identical to the evolution of the pure forcing run. This is because the forcing still dominates the dynamics in this case, whereas self-gravity becomes the dominant force in case SG64. Visual inspection of SG64 in comparison with pure forcing reveals that mixing of tracer particles occurs for both cases, but mixing is less efficient in the self-gravitating case. This is to be expected, since self-gravity acts to confine dense cores, within which the turbulent kinetic energy is less than the potential energy. Tracer particles located in such regions are trapped by self-gravity.

In order to quantify this behavior, we compare probability distribution functions (PDFs) of the Eulerian gas density (density defined on the grid) and PDFs of Lagrangian gas density (interpolated from the grid and monitored at the position of each tracer particle). In fully developed compressible turbulent flows, the PDF of density is close to a
Figure 4. Same as figure 3, but for the self-gravitating case SG64. The Lagrangian PDF of the tracer particles (solid line) as well as the Eulerian PDF (dashed line) deviate from a log-normal distribution at high densities and never fall on top of each other. In contrast to the case of pure forcing, complete mixing is impossible due to gravitational confinement. However, also in this case, turbulent transport to low-density regions is very efficient. The dotted lines are least-squares fits using the log-normal distribution given by equation (8).

The log-normal distribution e.g. (Klessen 2000, Kritsuk et al 2007, Li et al 2004, Ostriker et al 2001, Padoan et al 1997) and given by

\[ p_{v,m}(s) = \frac{1}{\sqrt{2\pi} \sigma} \exp \left[ -\frac{(s - s_{v,m})^2}{2\sigma^2} \right] ds, \tag{8} \]

with \( s \equiv \ln(\rho/\rho_0) \), mean \( s_{v,m} \) and variance \( \sigma^2 \). The subscripts \( v \) and \( m \) denote volume- and mass-weighted distributions, respectively. Volume- and mass-weighted PDFs are related by \( s_v = -s_m = -\sigma^2/2 \) (e.g. Li et al 2003). We make use of this fact to transform the volume-weighted log-normal Eulerian PDF into the corresponding mass-weighted PDF. This allows us to directly compare the Eulerian PDF with the Lagrangian PDF of the tracer particles, which is naturally a mass-weighted distribution.

Figure 3 shows the time sequence of the mass-weighted PDFs of both Eulerian (dashed lines) and Lagrangian (solid lines) gas density for the case of pure forcing. At \( t = 1.00T \), the tracer particle distribution covers densities in excess of \( s \approx 2.3 \), which corresponds to \( \log_10(\rho/\rho_0) \approx 1 \), as expected from their deposition criterion. The Eulerian distribution is in good agreement with a log-normal distribution, indicated by a fit using equation (8) (dotted line), which justifies our transformation from volume- to mass-weighted PDFs. Following the time sequence, it is evident that the tracer particle PDF converges to the Eulerian PDF. For \( t > 1.30T \), both Eulerian and Lagrangian distributions are (except for small fluctuations in the wings of the distributions) statistically identical. This behavior indicates mixing of tracer particles to rarefied lower density regions.

In contrast to the case of pure forcing, the PDFs from SG64 shown in figure 4 never reach a state where they resemble each other. Especially the high-density wings, which are mostly affected by self-gravity, deviate from a log-normal distribution. The Eulerian PDF tends to develop a power law tail for high densities, in agreement with Klessen (2000). Although significant mixing into low-density regions occurs within 0.1T of the tracer particle deposition, some tracers never completely mix with the background gas, owing to the self-gravity of the gas that holds them within deep gravitational potential wells in high-density regions. The onset of gravitational collapse manifests in the increasing probability for tracer particles to be found at very high density, which is indicated by the flattening of the Lagrangian PDF toward high density.

The fraction of tracer particles that have been mixed to regions of density smaller than their deposition density \( (\rho < 10\rho_0) \) can be estimated using cumulative distribution functions (CDFs) of the Lagrangian density distribution. We compare CDFs of all three runs (pure forcing, SG4 and SG64) at time \( t = 1.1T \) in figure 5. For the simulation without self-gravity and for SG4, approximately 95% of the tracer particles have been mixed to regions of density smaller than \( 10\rho_0 \) (vertical dashed line). In the case of ‘strong’ self-gravity (SG64), approximately 70% have been transported to low
density. This quantifies the influence of self-gravity in run SG64 on the mixing efficiency compared with pure forcing and SG4 cases. Although a significant fraction of tracer particles remains at high density, most of the tracer particles have already been mixed into lower density regions within 0.1 T after their deposition, even in case SG64.

4. Conclusions

Turbulent mixing of shock-compressed dense gas, which is associated with molecular hydrogen (H2) and followed by means of Lagrangian tracer particles has been investigated in self-consistent three-dimensional numerical simulations of driven supersonic turbulence. Even for self-gravitating media, turbulent transport from high-density cores to low-density rarefied regions is very efficient. Using Lagrangian tracer particles allowed us to directly confirm and quantify the importance of turbulent transport as the main mechanism for H2 mixing in the interstellar medium (see Glover and Mac Low 2007). We estimate that approximately 70% of the H2 formed in shock-compressed clumps and filaments can be mixed into lower density gas within one-tenth of a turbulent crossing time for a solenoidally driven turbulent medium. This represents an upper limit for the mixing timescale of 0.3 Myr for typical interstellar cloud conditions in the cold neutral medium (rms Mach number 3, cloud diameter 10 parsec, sound speed 0.6 km s\(^{-1}\), dimensions similar to Glover and Mac Low 2007). However, many sources of interstellar turbulence are likely to drive compressive modes directly, e.g. Galactic spiral density shocks, supernova explosions, gravity, protostellar jets and outflows. Therefore, the influence of using compressive forcing instead of the usually applied solenoidal forcing needs to be quantified in a follow-up study.

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