

Hydrodynamical Simulations of Molecular Dynamics in Supersonic Turbulent Flow

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Abstract. Here we present results from simulations of turbulence in star forming environments obtained by coupling three dimensional hydrodynamical models with appropriate chemical processes. We investigate regimes of decaying high-speed molecular turbulence. Here we analyse PDFs of density for the volume, mass, molecular mass and the energy distribution over the range of scales. We compare our results to those previously obtained for isothermal turbulence and suggest possible explanations.

Keywords: hydrodynamics – turbulence – molecular processes – clouds – ISM

1. Motivations

It is generally accepted now that supersonic turbulence is of fundamental importance to many processes related to the formation of stars (Vázquez-Semadeni et al., 2000; Padoan et al., 2001; Mac Low and Klessen, 2003). Turbulent motions redistribute energy inside molecular clouds, giving rise to their hierarchical structure and determining cloud fragmentation (Padoan and Nordlund, 2002). In this article we report results of our ongoing study of molecular turbulence, i.e. turbulence in the fluid with active chemistry and cooling appropriate for the star-forming environments.

Molecular chemistry and cooling is critical to cloud formation and evolution (Langer et al., 2000; Lim, 2001; Lim et al., 1999). Molecular hydrogen forms most efficiently where the gas is warm but the grains are cool (H_2 forms mainly when atoms combine after colliding and sticking to dust grains). Simple molecules like OH, CO and H_2O form in the gas phase with H_2 as the reactive agent. These molecules are not only important coolants, but associated emission lines provide a means

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of measuring the cloud properties. Molecules are dissociated as a consequence of fast shocks, UV radiation, X-rays and cosmic rays (Herbst, 2000). We thus need to study molecular turbulence to determine the distribution and abundances of molecular species.

1.1. METHODS

Numerically we solve the time-dependent flow equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (1a)$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p, \quad (1b)$$

$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \nabla e = -p \nabla \cdot \mathbf{v} + \Lambda(T, n, f), \quad (1c)$$

$$\frac{\partial (fn)}{\partial t} + \nabla \cdot (fn\mathbf{v}) = R(T, n, f) - D(T, n, f), \quad (1d)$$

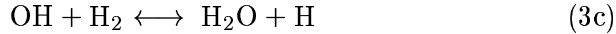
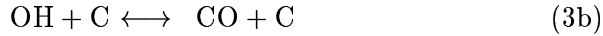
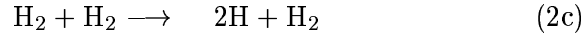
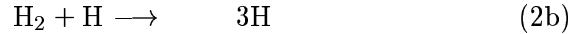
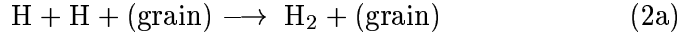
where n is the hydrogen nuclei density, e is the internal energy density and f is the molecular hydrogen abundance (i.e. $n(\text{H}_2) = fn$). We consider the gas as a mixture of atomic and molecular hydrogen with 10% of helium (i.e. $n(\text{He}) = 0.1n$), therefore the total particle density is $n_{tot} = (1.1 - f)n$ and the temperature is $T = p / (k n_{tot})$. Λ is internal energy loss through radiation and chemistry per unit volume, the function consists of 13 separate parts (some of which heat the gas), their detailed description can be found in Smith and Rosen, Pavlovski et al. (2003, 2002). R and D are reformation and dissociation rates of molecular hydrogen respectively (see Appendix A and B in Smith et al., 2002).

As a basis, we employ the ZEUS-3D code (Stone and Norman, 1992). This is a second-order in space and first order in time, grid-based code, which is using van Leer type advection. We study here compressible hydrodynamics without external gravity, self-gravity or thermal conduction. A small amount of linear physical viscosity is modelled, and von Neumann type of artificial viscosity used to capture shocks and determine the dissipation in the shock front.

For computation of cooling we have employed the simultaneous implicit method discussed by Suttner et al. (1997) in which the time step is adjusted so as to limit the change in internal energy in any zone to 30%. This limit implies much shorter time-steps in comparison to any dynamical timescale, and it is one of the most restraining factors in our simulations.

The cooling is appropriate for dense cloud material of any atomic-molecular hydrogen mixture. We include H₂ ro-vibrational and dissociative cooling, CO and H₂O ro-vibrational cooling, gas-grain, thermal bremsstrahlung and a steady-state approximation to atomic cooling (see Appendix A of Smith et al., 2002 and Pavlovski et al., 2002).

We take a very basic network of chemical reactions. Time-dependent hydrogen chemistry is included (Eqns. 2a,b,c), but C and O chemistry is limited to the reactions with H and H₂ which generate OH, CO and H₂O (Eqns.3a,b,c). Equilibrium abundances are calculated, which are accurate for our purposes within the shocks where molecules are rapidly formed and destroyed.



2. Simulations

We have run a set of simulations (with resolution ranging from 32^3 to 256^3) of *decaying* turbulence in different velocity regimes: 15 km s^{-1} , 30 km s^{-1} , 60 km s^{-1} . The number density has been taken to be $n = 10^6 \text{ cm}^{-3}$, physical box size $L = 10^{16} \text{ cm}$, and the initial temperature has a homogeneous distribution of $T_0 = 100 \text{ K}$. The hydrogen was fixed to be *fully molecular* at the beginning: fraction $f = 0.5$. The high number density was selected to create a sufficiently high average column (10^{22} cm^2), which ensures that the simulated region is optically thick. Initial stress was introduced by perturbations applied to model velocities with a spectrum extending over a narrow range of wave numbers $3 \leq |\mathbf{k}| \leq 4$ (see Fig. 1)

2.1. RESULTS

We find that the dynamical behaviour of the molecular turbulence is not dramatically different from behaviour of the turbulence with the isothermal equation of state.

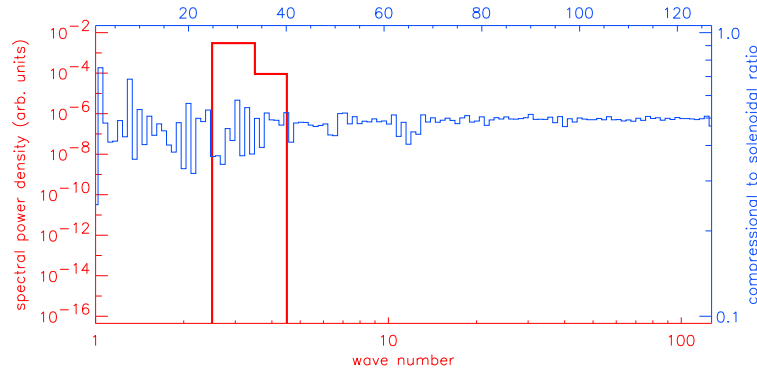


Figure 1. Initial energy distribution over the different scales. Thick line – total energy, corresponds to l.h.s. y-axis and bottom x-axis; thin line – ratio of the compressional to the solenoidal energy, corresponds to the r.h.s. y-axis and upper x-axis.

The decay law of kinetic energy in the simulations are similar to the decay laws of the high Mach number isothermal simulations uncovered in Smith et al. (2000). However, in our simulations thermal energy is not constant, and decays only a little bit slower than kinetic energy (for full details see Pavlovski et al., 2002). This fact results in sustaining Mach number > 1 for a longer, compared to isothermal regime, time.

Statistical analysis of the turbulence showed that probability density functions (PDFs) of fractional volume per unit density ($dV/d\rho$), fractional mass per unit density ($dM/d\rho$), and fractional molecular mass per unit density ($d\mathfrak{M}/d\rho$) can be approximated by log-normal distributions as in the isothermal case (Padoan et al., 1997; Passot and Vázquez-Semadeni, 1998; Ostriker et al., 2001),

$$p_{V,M,\mathfrak{M}}(\log(x)) = \frac{1}{\sigma_{V,M,\mathfrak{M}}\sqrt{2\pi}} \exp\left\{-\frac{(\log(x) \pm |\mu_{V,M,\mathfrak{M}}|)^2}{2\sigma_{V,M,\mathfrak{M}}^2}\right\}, \quad (4)$$

where $x = \rho/\langle\rho\rangle$, $\langle\rho\rangle$ – volume mean of density. We find, that modules of means for the distribution have close values, but generally the following is true:

$$|\mu_V| \lesssim |\mu_M| \lesssim |\mu_{\mathfrak{M}}|, \quad \sigma_V > \sigma_M \gtrsim \sigma_{\mathfrak{M}}. \quad (5)$$

Typical distributions of these values are presented in Figs. 2,3. The values of the parameters of the distributions are: in the isothermal case, $\mu_V = -0.43$, $\mu_M = 0.47$, $\sigma_V = 0.74$, $\sigma = 0.51$; in the molecular case,

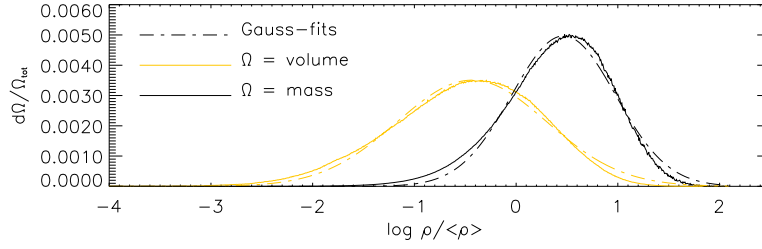


Figure 2. PDFs of volume and mass distributions with density in the initially high speed isothermal turbulence. Data taken from 256^3 simulations with initial r.m.s. velocity of 60 km s^{-1} after 130yr of evolution (average Mach number: $\mathcal{M} \approx 9$)

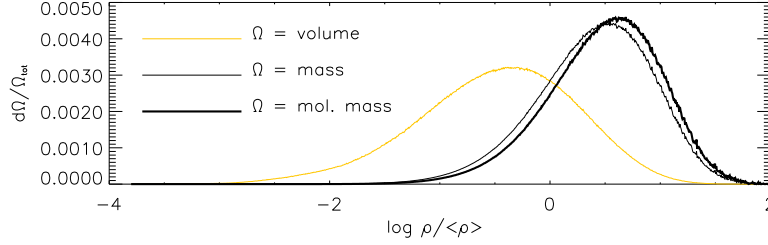


Figure 3. PDFs of volume, mass and molecular mass distributions with density in the decaying molecular turbulence. Data taken from 256^3 simulations with initial r.m.s. velocity of 60 km s^{-1} after 130yr of evolution (average Mach number: $\mathcal{M} \approx 10$)

$\mu_V = -0.42$, $\mu_M = 0.46$, $\mu_{\text{mol}} = 0.55$, $\sigma_V = 0.71$, $\sigma_M = 0.52$, $\sigma_{\text{mol}} = 0.50$. This is in agreement with the results discussed in Ostriker et al. (2001).

2.2. MOLECULAR HYDROGEN EVOLUTION

The molecular fraction ‘ f ’ is displayed in Fig. 4. The three initial states correspond to three distinct physical regimes. With a r.m.s. velocity of 15 km s^{-1} , dissociative shocks are not present but some localised dissociation still occurs. With 30 km s^{-1} , a few per cent of the molecules are dissociated whereas at 60 km s^{-1} , the gas becomes over 80% atomic.

Reformation of molecular hydrogen is unexpectedly rapid. The expected H_2 reformation time at 20 K and 10^6 cm^{-3} is $t_R = 3,200 \text{ yr}$ (see details in Pavlovski et al., 2002) a factor of 5 larger than the simulation time. At 100 yr , the temperature is $\sim 80 \text{ K}$, predicting a reformation time of $t_R = 2,000 \text{ yr}$. Yet, reformation is occurring over $\sim 400 \text{ yr}$. This speed up is caused by the turbulence itself: the molecules preferentially reform in the denser and cooler locations. As weak shocks propagate through the gas, different regions are compressed and expanded. Hence the reformation time is not only controlled by the ‘average’ reformation

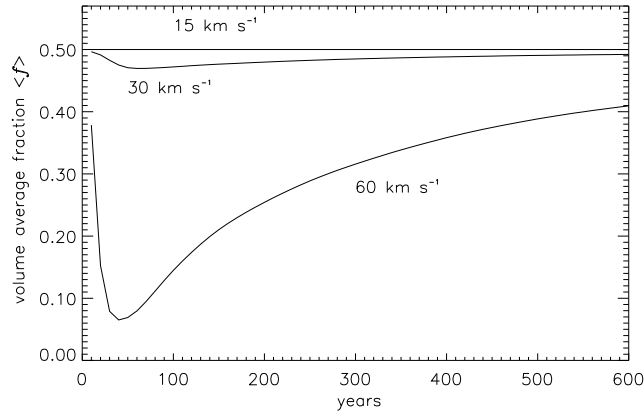


Figure 4. Evolution of the average molecular fraction with time in the runs with different initial r.m.s. velocity. Data from the 256^3 runs.

time, but also by the strength of the turbulence. Given a turbulent dynamical timescale shorter than the average reformation timescale, then we can expect reformation to be accelerated.

3. Summary

We have presented the properties of a specific model for molecular turbulence. We carried out three dimensional hydrodynamical simulations of decaying supersonic turbulence in molecular gas. We included a detailed cooling function, molecular hydrogen chemistry and equilibrium C and O chemistry. We studied three cases in which the applied velocity field straddles the value for which wholesale dissociation of molecules occurs. The parameters chosen ensure that for the high-speed turbulence, the molecules are initially destroyed in shocks and gradually reform in a distinct phase.

We find the following.

- An initial phase of slow dissipation and shock formation.
- An extended phase of power-law kinetic energy decay, as in the isothermal case.
- The thermal energy, initially raised by the introduction of turbulence, decays only a little slower than the kinetic energy.
- The reformation of hydrogen molecules, as the fast turbulence decays, is several times faster than expected from the average density.

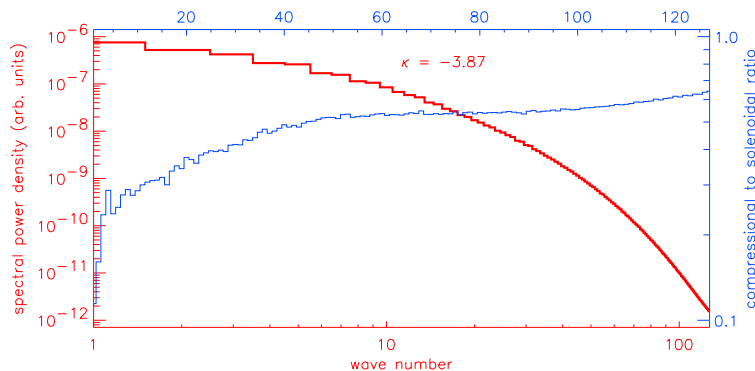


Figure 5. Distribution of energy over different scales at the end of the simulation (600 yr: 60 km s^{-1} , 256^3). Thick line – total energy, corresponds to l.h.s. y-axis and bottom x-axis; thin line – ratio of the compressional to the solenoidal energy, corresponds to the r.h.s. y-axis and upper x-axis. Steeper than Kolmogorov’s ($-11/3$) energy cascade as indication of strong dissipation.

- The molecular fraction increases quite uniformly, so that density and molecular density are almost identically distributed at any one time.

We mainly wish here to emphasise the insight these simulations provide into how molecular chemistry and supersonic dynamics combine. We have found that isothermal simulations are indeed very useful, not only for the rate of energy decay but also to trace the molecules.

A simple reason for the fast decay is that a sufficient number of strong shocks survive. As shown by Smith et al. (2000), the rate of energy decay in *decaying* turbulence is dominated by the vast number of weak shocks. These shocks are less efficient at energy dissipation. A second possible reason is that the curved shock structures create small scale vorticity, which leads to enhanced dissipation of kinetic energy. The latter argument is supported by the fact that the energy distribution is steeper than that of Kolmogorov’s spectrum, see Fig. 5

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