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The role of turbulence in the chemical evolution of the interstellar medium.

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Abstract

Turbulence is ubiquitous in the interstellar medium (ISM) and can introduce large variations in the density field of molecular clouds. However, the vast majority of chemical models for the ISM can only assume a constant gas density based on line-of-sight averaged observations. In order to assess the impact of these variations of the gas density in the chemical evolution of the ISM, we are conducting a series of magnetohydrodynamical (MHD) numerical simulations of different phases of the ISM with `Athena++`; the resulting three-dimensional distributions of gas are then used to compute the chemical evolution of the system using the code `Nautilus`. In this contribution, we present the first results of our study focused on the chemistry of a molecular cloud filament.

1 Introduction

Observational studies of the chemistry of the interstellar medium (ISM) rely on state-of-the-art chemical codes that, provided a given number of input parameters such as gas and dust temperatures, hydrogen particle number, visual extinction, cosmic ray ionisation rate, the intensity of the local ultraviolet radiation field, and the dust to gas ratio, compute the expected chemical abundances $n_{\rm X}/n_{\rm H}$ of a set of molecules X (CO, HCO^+, N_2H^+, etc.) based on a huge amount of chemical reactions [6, 8]. However, sometimes the predictions made by the models do not match the observations, and it is in fact very complicated to fit all the molecular species to the same chemical model [3]. Appart from the limitations imposed by the observing facilities, the cause of this mismatch between observations and predictions may rely on the chemical networks, input parameters and underlying approximations. The chemical reactions involved in the chemical networks are being revised in laboratories in order to improve the accuracy of the binding energies, although so far only rough estimates have been set with large uncertainties [7]. Therefore, as a complement to laboratory experiments, it seems reasonable to explore to what extent the input parameters might explain the deviations of the predictions from the expectations. In this work, we have focused on two key elements

that drastically affect the predicted abundances: the hydrogen number density and the dust-to-gas ratio.

resulting chemical model and its predictions has been shown, for instance, by [3]. On the other hand, several recent numerical studies have shown that the dust-to-gas ratio is not constant due to turbulent motions of the gas and the decoupling of dust grains as a result of their net charge and their interaction with the ambient magnetic field; these variations of the dust-to-gas ratio are present in all regimes of the ISM, from the diffuse ionised envelopes of molecular clouds [1] to their cool interiors [5] (see Fig. 1).

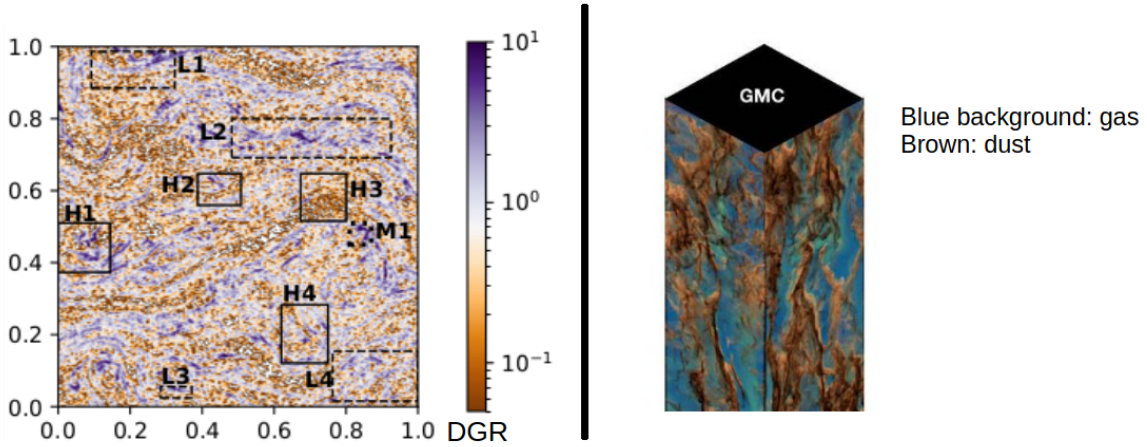

Figure 1: Examples of variations of the dust-to-gas ratio in simulations of the ISM. *Left*: dust-to-gas ratio map for a 2D simulation of a molecular cloud envelope [1]. *Right*: dust (brown) and gas (blue) distribution on a 3D simulation of a giant molecular cloud [5].

In consequence, we want to explore two possible reasons for the mismatch between observations and predictions of chemical models: small-scale density variations caused by turbulence at scales not resolved by telescopes, and variations of the dust-to-gas ratio that affect the abundances of solid-phase formed species. In this contribution we present our results for the first part, the one centred on the effects of turbulence on the predicted chemical abundances. The effects of the variations of the dust-to-gas ratio are going to be assessed in future publications.

2 Chemistry and MHD simulations

In order to recreate the turbulent state of a molecular cloud, we run a simulation with the `Athena++` code [9] in three dimensions under the assumption of isothermal, ideal MHD with periodic boundary conditions and at a resolution of 256^3. We assume a molecular hydrogen particle density $n_{\mathrm{H_2}} = 2.57 \times 10^4$ cm^{-3} with a magnetic field parallel to the x-axis and a strength of $B_0 = 40$ μG. We take a medium initially at rest to which we continuously inject turbulence until the energy injection rate equals the dissipation rate, a point at which we as-

sume we reproduce the steady state of a trans-sonic molecular filament (which is compatible with the interior of a molecular cloud before collapse, see [4]). Although this simulation is dimensionless, for the discussion we always consider a nominal length for our box of 0.05 pc, which is small enough to contain from two to three beams of IRAM 30 m telescope at frequencies between 80 GHz and 200 GHz.

As a consequence of turbulence, we obtain large deviations of the initial gas density of $n_{H_2} = 2.57 \times 10^4$ cm^{-3}, by a factor of up to two orders of magnitude (see Fig 2); regions with high and low gas density share their sheet-like morphology and are extended along the mean magnetic field direction (x-axis). If we take these hydrogen densities and assume a constant gas and dust temperature of $T = 12$ K, a visual extinction $A_V = 4$ mag and a cosmic ray ionisation rate of $\zeta = 5 \times 10^{-17}$ s^{-1}, and retrieve the predicted chemical abundances of the commonly studied molecules with the `Nautilus` code [8] at an age of 10^6 yr (see Fig. 2), we see that turbulence is bound to produce notable differences in the observed abundances of some species, especially CO.

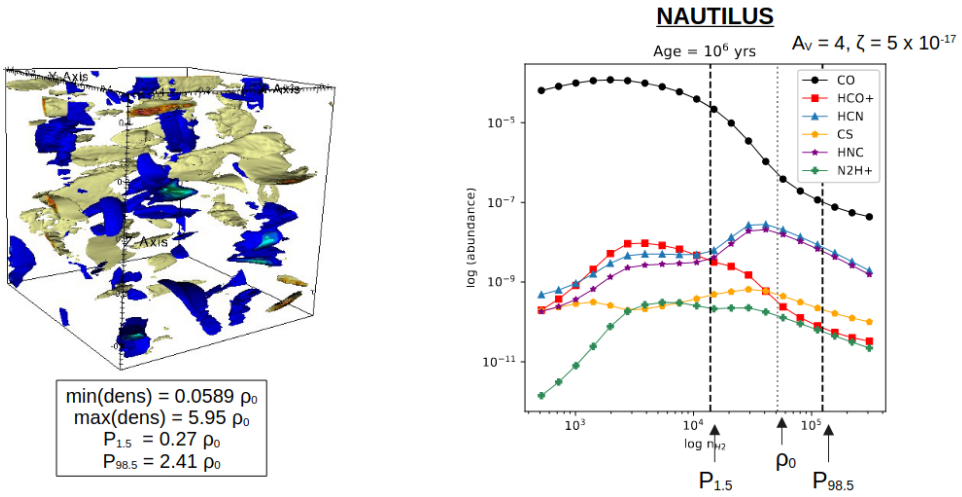

Figure 2: *Left*: gas structures present in the steady state simulation. Low-density structures are those below the 1.5 % of the density distribution and are coded in yellow. High-density structures are selected based on the 98.5 % threshold and are coded in blue. *Right*: chemical abundances predicted by `Nautilus` in the density range of the steady state simulation. The vertical dotted line corresponds to the initial density, while the dashed lines correspond to the 1.5 % and 98.5 % density percentiles used in the left panel.

3 Observational expectations

Using the chemical network shown in Fig. 2, we have estimated for each simulation cell the expected abundance of the considered molecules using a linear interpolation in log-space density bins. With that, we have used the MHD cubes that provide the gas velocity field and gas distribution, together with the molecule distribution, and have applied the radiative

transfer code RADMC-3D [2] to obtain the spectra of rotational transitions. In Fig. 3 we show the molecular hydrogen column density map projected onto one of the faces of the 3D cube (xy plane, with the magnetic field parallel to the x-axis and, therefore, perpendicular to the line of sight) together with the predicted integrated intensity maps for ^{13}CO ($1 \rightarrow 0$) and CS ($2 \rightarrow 1$). Note that the range of integrated intensities is much wider for ^{13}CO ($1 \rightarrow 0$) (of the order of 0.4 K km s^{-1}) than for CS ($2 \rightarrow 1$) (of the order of 0.2 K km s^{-1}).

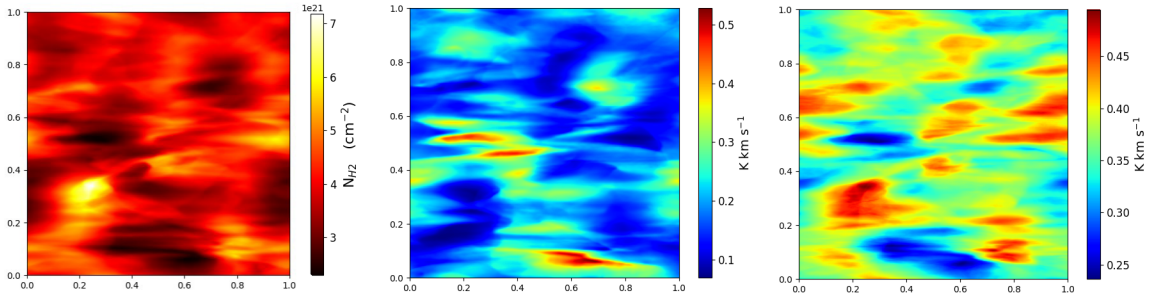

Figure 3: Molecular hydrogen column density (left) for the xy face of the cube, and the RADMC-3D predicted moment-zero maps for ^{13}CO ($1 \rightarrow 0$) (middle panel) and CS ($2 \rightarrow 1$) (right panel).

When trying to fit a chemical model to observations, a common assumption is to consider that the hydrogen density along the line of sight is constant, *i.e.* that the gas distribution is uniform. In order to quantify the effects of this assumption, we have post-processed with RADMC-3D a cube with uniform molecular hydrogen density and chemical abundances, and have computed the ratio between the turbulent case shown in Fig. 3 and the uniform ones. The results are shown in Fig. 4 in the form of relative integrated intensity maps and histograms of relative integrated intensities. In general, we see that the expectations raised in the view of the chemical network shown in Fig. 2 are in agreement with the results: turbulence produces large variations in the local abundance of ^{13}CO ($1 \rightarrow 0$), and can produce integrated intensities six times higher than when assuming a uniform gas distribution along the line of sight. On the other hand, other molecules are less sensitive to turbulence and the variations introduced are of the order of $10 - -20\%$, as is the case for CS ($2 \rightarrow 1$).

4 Summary and conclusions

In this contribution, we have presented the preliminary results of our study on the effects of turbulence on the chemistry of molecular clouds. Assuming a hydrogen particle density of $n_{\mathrm{H_2}} = 2.57 \times 10^4$ cm^{-3} and a magnetic field of $B_0 = 40$ μG, we have run an ideal MHD 3D turbulent box simulation with `Athena++` until we reproduce a steady-state molecular filament before collapse. Later, we have post-processed this simulation with the chemical code `Nautilus` in order to derive a cube of chemical abundances that has been used to estimate the molecular emission with RADMC-3D. We have compared the results of this post-processed turbulent simulation with the case where the gas density and the chemical

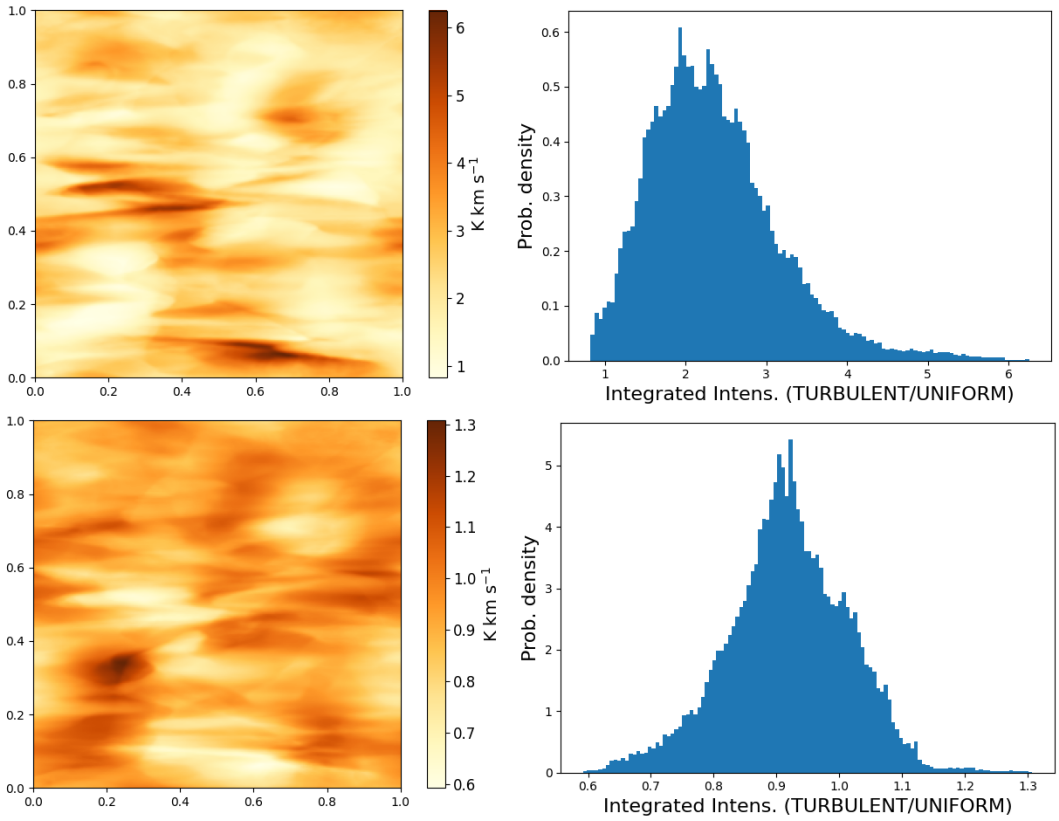

Figure 4: Relative integrated intensity maps and associated histograms for ^{13}CO ($1 \rightarrow 0$) (upper row) and CS ($2 \rightarrow 1$) (lower row). Note the significant differences between both molecules.

abundance are uniform along the line of sight. The results of this preliminary study can be summarised as follows:

- Turbulence can generate important density fluctuations – in this case from 0.05 to 6 times the mean value. Inside this range of densities, the chemical abundance of some elements present critical variations (especially CO).

- These density fluctuations are translated into variations in the moment-zero maps, which are especially important for ^{13}CO ($1 \rightarrow 0$) where the integrated intensities can be up to a factor of 6 higher than for the uniform case. Other molecules, such as CS ($2 \rightarrow 1$), are less affected by turbulence, although the difference in integrated intensities are of the order of a $10 - -20\%$.

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