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CONSEQUENCES OF WARM H_2 ON THE CHEMISTRY OF DIFFUSE MOLECULAR CLOUDS: THE CASE OF CH^+

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Abstract. The large abundances of CH^+ observed in the local diffuse interstellar gas have been a longstanding problem. The main formation path is the ion-neutral reaction between C^+ and H_2, which is highly endothermic. This reaction requires either warm reactants or non-thermal processes to occur efficiently. Our main goal is to evaluate the relative roles of the presence of warm H_2, and the increased formation rate due to the ion-neutral drift in the production of CH^+. We performed a hybrid approach using magnetohydrodynamical simulations with the RAMSES code, where the formation of H_2 is included, along with a post-treatment of the chemistry. We explore the role of the cosmic ray ionisation rate on the chemistry. We find that the warm H_2 is a key ingredient in the formation of CH^+

Keywords: ISM: clouds, CH^+, H_2, Methods:numerical

1 Introduction

Molecular clouds display a wide range of physical conditions, where the two main phases known as warm neutral medium (WNM) and the cold neutral medium (CNM) coexist at pressure equilibrium (Field 1965). Turbulent motions within molecular clouds have a multifaceted role. They create density fluctuations, where the chemistry can proceed faster, they intermingle the two phases maintaining gas in the thermally unstable phase (Audit & Hennebelle 2005), and they transport long-lived molecules to environments where they are not expected to be produced. This is the case of molecular hydrogen (H_2) which can be produced in transitory cold and dense structures created by the turbulence, and then trasported to warmer regions where it is shielded by the structure of the molecular cloud (Valdivia et al. 2016c). Such warm H_2 can eventually participate in endothermic reactions.

An interesting related problem is the formation of CH^+, which requires molecular hydrogen to be formed efficiently. CH^+ has been observed in the interstellar medium (ISM) of our galaxy in visible wavelenghs (Crane et al. 1995; Gredel 1997; Weselak et al. 2008), and $^{13}CH^+$ has been detected deeper in the Galactic disc in infrared wavelengths (Falgarone et al. 2005, 2010; Godard et al. 2012). In the diffuse ISM, CH^+ is easily destroyed by reactions with electrons, hydrogen atoms and hydrogen molecules, and the only reaction able to efficiently produce CH^+ under such conditions is

$$C^+ + H_2 \rightarrow CH^+ + H \qquad (\Delta E/k = -4300\ K), \tag{1.1}$$

which is a highly endothermic ion-neutral reaction (Agúndez et al. 2010). Two effects can increase the efficacity of this reaction. The first one is the presence of warm reactants, or in other words, the presence of warm H_2, and the second one is the drift between neutrals and ions (Myers et al. 2015).

2 Numerical methods

In order to evaluate the importance of these two effects under realistic conditions, we post-process a high-resolution magnetohydrodynamical (MHD) multiphase simulation of a molecular cloud, where the formation

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and destruction of H_2, as well as the thermal feedback, are included (Valdivia et al. 2016c). The dust and H_2 selfshieldings are estimated using our tree-based method (Valdivia & Hennebelle 2014). We post-process a snapshot (at 15 Myr) using a chemical solver that we developed (Valdivia et al. 2016b), which is able to prescribe the H_2 abundance, while computing the rest at equilibrium. The validity of our approach is justified in a companion work (Valdivia et al. 2016a).

3 Results

3.1 Role of warm H_2

To assess the importance of warm H_2 in the abundance of CH^+ we calculate the abundance of CH^+ in two ways. In the first case we calculate the chemical equilibrium by fixing the H_2 abundance to the value obtained in the simulation (out-of-equilibrium), while in the second case we do it for all the species, including H_2. The left panel of Fig. 1 shows that the out-of-equilibrium H_2 found at the edge of the clumps locally increases the abundance of CH^+ up to 2-3 orders of magnitude. The panel on the right shows that the integrated column densities are 3-10 times higher than those obtained when H_2 is considered to be at equilibrium.

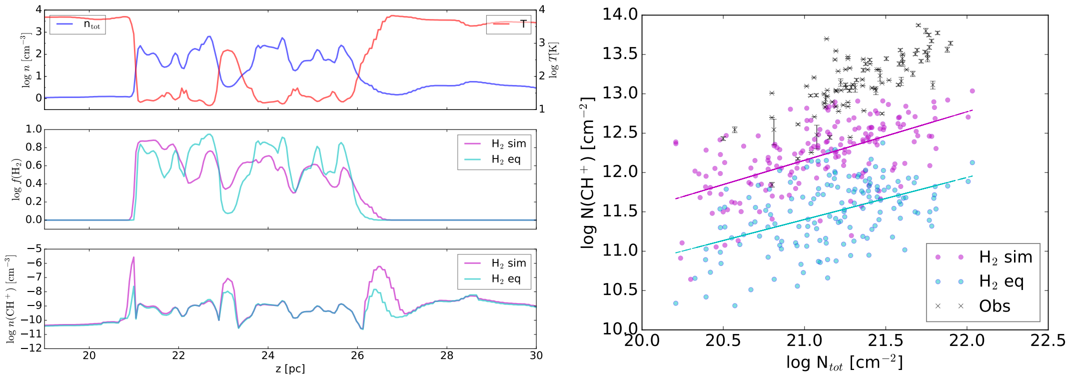

Fig. 1. Left: Line-of-sight showing the effect of warm H_2. From the top to the bottom panels show the density and temperature, the H_2 fraction obtained from the simulation and what is expected at equilibrium, and the associated CH+ number density. **Right:** Comparison of the column densities of CH^+ as a function of the total column density obtained for the case when H_2 is fixed from the simulation and for the case where it is calculated at equilibrium. The crosses are the observational data (Crane et al. 1995; Gredel 1997; Weselak et al. 2008).

3.2 Role of the ion-neutral drift

The drift between ions and neutrals can increase the reaction rate of highly endothermic ion-neutral reactions, acting as an increase of the effective temperature $T_{\rm eff}$ (Draine 1980; Draine et al. 1983; Flower et al. 1985):

$$T_{\rm eff} = T + \Delta T; \qquad \Delta T = \frac{\mu}{3k} v_{\rm d}^2, \tag{3.1}$$

where T is the gas temperature, and the increase in temperature ΔT depends on the ion-neutral drift velocity $v_{\rm d}$. In this expression μ is the reduced mass for the reaction, and k is the Boltzmann constant. The reaction rate of the ion-neutral drift is proportional to $\exp(-\max\{\beta/T_{\rm eff}, (\beta - 3\Delta T)/T\})$.

As our simulation is ideal, the ion-neutral drift velocity is estimated from the balance between the Lorentz force with the ion-neutral drag as

$$v_{\rm d} \approx \frac{(\nabla \times \vec{B}) \times \vec{B}}{4\pi \sum_{jk} n_j n_k \mu_{jk} K_{jk}} \tag{3.2}$$

where $\vec{B}$ is the magnetic field, n_j and n_k are the number densities of the neutral and ionic species, μ_{jk} is the reduced mass and K_{jk} is the momentum transfer coefficient of species j and k. We consider H, H_2 as the neutral species, and H^+, He^+, C^+, and S^+ as the ionic species. For the momentum transfer coefficients we use the values of Pinto & Galli (2008), and the Langevin rates whenever more accurate expressions were not available.

Figure 2 shows the distribution of ion-neutral drift velocities obtained for our simulation, which peaks around 0.04 km s^{-1}, with a tail that decays very fast for high velocities, producing a negligible effect on the effective temperature distribution, as shown in the central panel of the same figure. The effect on the abundance of CH^+ is also negligible, as shown in the right panel in Fig. 2.

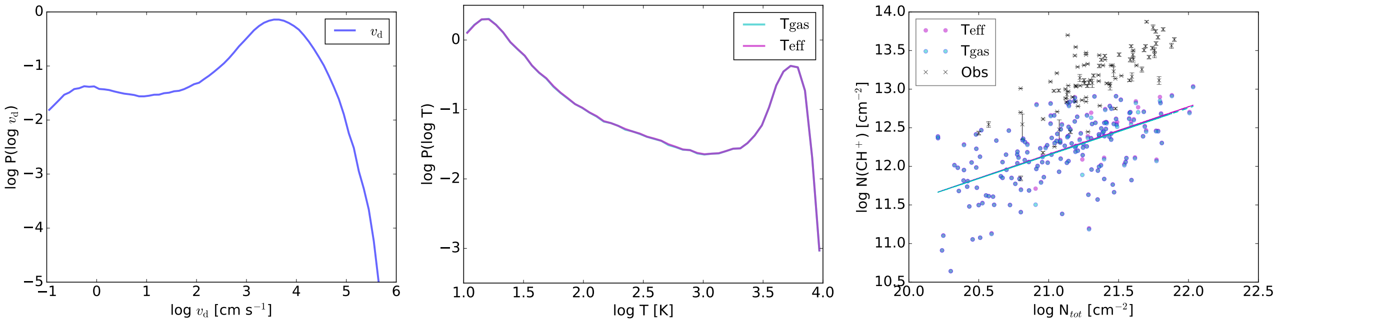

Fig. 2. Left: Normalised volume-weighted drift velocity distribution obtained for our simulation. **Centre:** Normalised mass-weighted distribution of the gas temperature and the effective temperature. **Right:** Comparison of the column densities of CH^+ as a function of the total column density for the cases where the ambipolar diffusion is not included and including this effect.

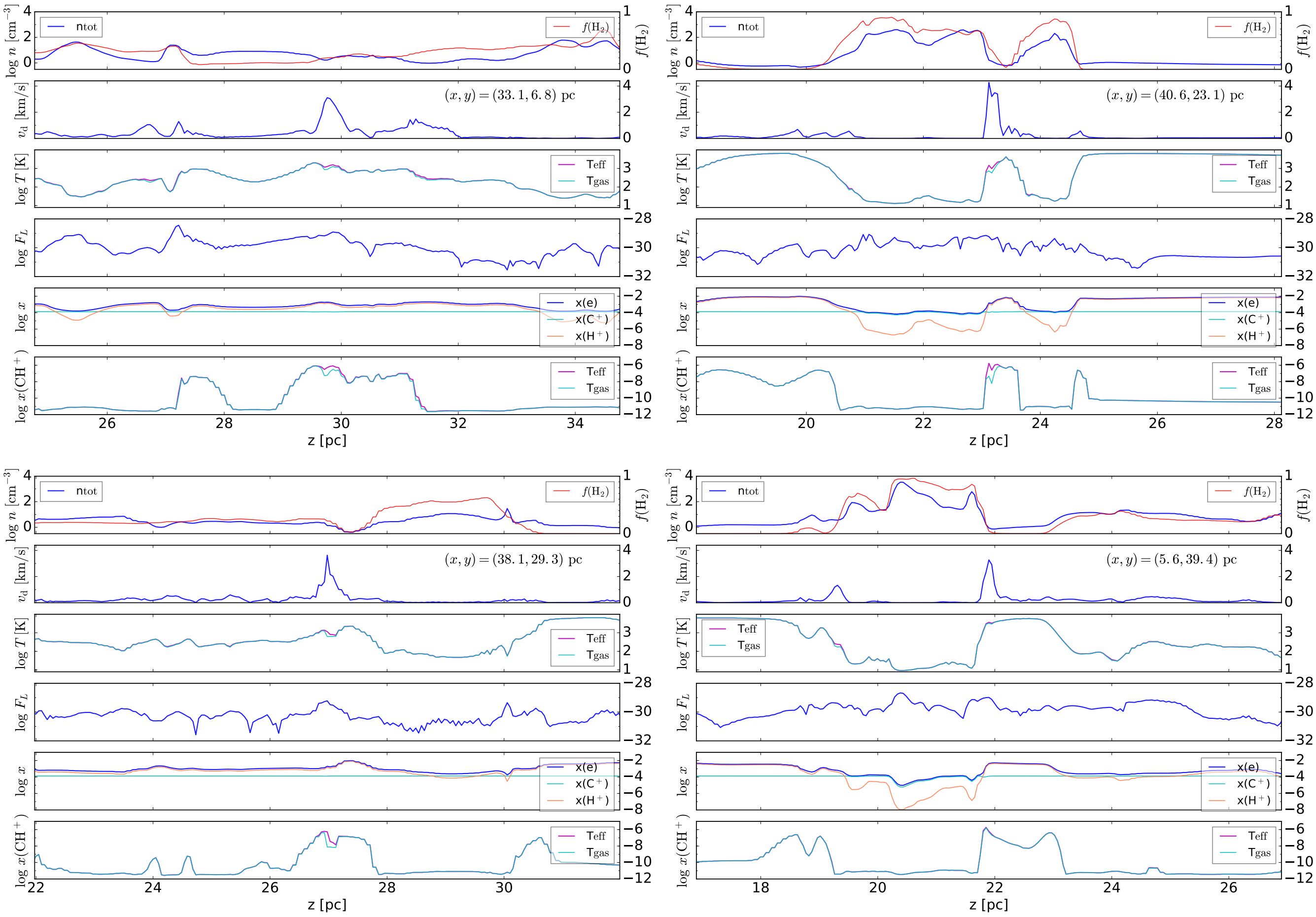

Fig. 3. Lines-of-sight with high ion-neutral drift velocities. Each panel shows (from the top to the bottom) the total number density and the H_2 fraction, the drift velocity, the gas temperature and the effective temperature, the Lorentz force, the electronic fraction, and the CH^+ abundance.

To better see the effect of the ion-neutral drift, we select four lines of sight that present drift velocities of at least 3 km s^{-1}, shown in Fig. 3. These lines-of-sight show that high drift velocities arise in low density and warm gas, as expected from Eq. 3.2. These regions of high v_d are very localised, and the ion abundance is close to $10^{-3} - 10^{-2}$ and dominated by H^+. Despite producing small differences in the effective temperature, the ion-neutral drift can locally increase the abundance of CH^+ up to one order of magnitude. Unfortunately, regions with high drift velocities are very uncommon and thus the effect is negligible.

3.3 Role of the cosmic ray ionisation rate

Cosmic rays can alter the chemistry of the ISM by producing species such H^+, He^+, and H_2^+, that can participate in ion-neutral reactions, which proceed at rates much faster than reactions between neutrals. Even though our simulation uses a cosmic ray ionisation rate of $\zeta = 3 \times 10^{-16}$ s^{-1}, we explore the role of different values of ζ in our post-processing for the chemistry. The left panel of Fig. 4 shows the results for a line-of-sight for three different values of $\zeta = 3 \times 10^{-17}, 3 \times 10^{-16}$, and 3×10^{-15} s^{-1}. This line-of-sight shows that even though the ion fraction increases for higher values of ζ, the abundance of CH^+ is less sensitive. However, the variation in CH^+ is systematic, and smaller values of the cosmic ray ionisation rate can slightly increase the CH^+ abundances.

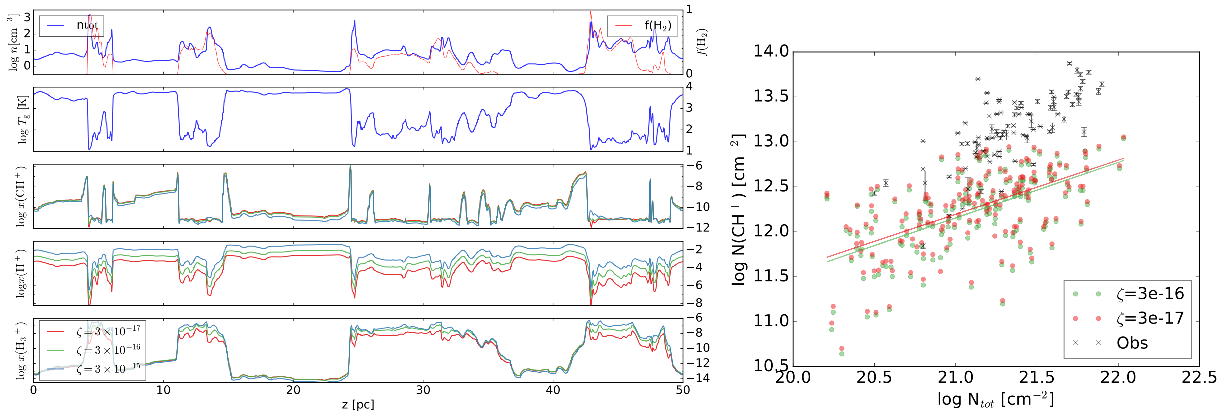

Fig. 4. Left: Line-of-sight showing the effect of the cosmic ray ionisation rate ζ. **Right:** Comparison of the column densities of CH^+ as a function of the total column density for two values of ζ. In both cases the values of ζ are given in s^{-1}

4 Conclusions

Out-of-equilibrium (warm) H_2 is crucial to form CH^+ efficiently in the diffuse ISM, nevertheless it is not enough to explain the observed abundances. High ion-neutral drift velocities can boost the CH^+ formation, but as these events are extremely rare, at least at the resolution of our simulation, the global effect of our distribution of v_d is statistically negligible. Nevertheless, as our simulation lacks of a description of small scale processes, such as the intermitent dissipation of energy or ambipolar diffusion, future works must address this issue. The cosmic ray ionisation rate has a moderate impact on the abundance of CH^+, but it can play a central role on the abundances of other species.

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