The Hydride Toolbox

Origin Of CH⁺ In Diffuse Molecular Clouds

Outline

1. CH⁺ in the diffuse ISM
2. Hybrid approach for the chemistry
3. Warm H₂ and ion-neutral drift
4. Summary

V. Valdivia, B. Godard, P. Hennebelle, M. Gerin, P. Lesaffre, and J. Le Bourlot

(A&A in press)

valeska.valdivia@cea.fr
UPMC-Paris December 2016
• Simple hydride

• Easily \textit{destroyed}

• Main formation path is \textit{highly endothermic}
  \[ \text{C}^+ + \text{H}_2 \rightarrow \text{CH}^+ + \text{H} \quad (\Delta E/k = -4300 \text{ K}). \]

• Classical PDR models predict low abundances in the diffuse ISM

• But observations reveal \textit{relatively high abundances}
Impact of the turbulent mixing CNM/WNM on the chemistry
Impact of the multiphase structure
**PDR Models**

- Stationary plane-parallel slabs illuminated from one or two sides

**Dissipation of Turbulence**

- Burst of dissipation
  - L~10 AU ; t~100 yr

**Ion-Neutral Drift**

\[ T_{\text{eff}} = \frac{m_i T_n + m_n T_i}{m_i + m_n} + \Delta T \]
\[ \Delta T = \frac{\mu v_d^2}{3k} \]

<table>
<thead>
<tr>
<th>( N_{\text{CH}^+} ) (10^{13} cm(^{-2}))</th>
<th>( N_H ) (10^{21} cm(^{-2}))</th>
<th>( v_{d,99} ) (km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>2.2</td>
<td>2.1</td>
</tr>
<tr>
<td>0.8</td>
<td>2.2</td>
<td>3.0</td>
</tr>
<tr>
<td>1.1</td>
<td>1.2</td>
<td>2.3</td>
</tr>
<tr>
<td>0.9</td>
<td>1.3</td>
<td>2.2</td>
</tr>
<tr>
<td>0.6</td>
<td>1.9</td>
<td>1.7</td>
</tr>
<tr>
<td>1.4</td>
<td>2.0</td>
<td>2.5</td>
</tr>
<tr>
<td>1.6</td>
<td>1.9</td>
<td>2.2</td>
</tr>
<tr>
<td>1.2</td>
<td>2.7</td>
<td>1.9</td>
</tr>
</tbody>
</table>

**Other approaches:**

- Alfvén waves (Federman et al. 1996), Low velocity C-shocks (Draine & Katz 1986), Irradiated low-v C-shocks (Lesaffre et al. 2013)
On-the-fly

- Crucial species for the chemistry: \( \text{H}_2 \) which is a **bottleneck** for the chemistry.

\[
\frac{\partial n_{\text{H}_2}}{\partial t} + \nabla \cdot (n_{\text{H}_2} \mathbf{v}) = k_{\text{form}} n(n - 2n_{\text{H}_2}) - k_{\text{ph}} n_{\text{H}_2}.
\]

- Heating: PE, CR, \( \text{H}_2 \) (formation and destruction)

- Use cooling functions: CII, OI, Ly\( \alpha \), Rec, \( \text{H}_2 \)

- Compute dust shielding and \( \text{H}_2 \) self-shielding

\[
f_{\text{sh, H}_2} = < e^{-\tau_{d,1000}} f_{\text{shield}} >
\]

- Solve ideal MHD equations.

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0, \\
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} - \mathbf{B} \mathbf{B}) + \nabla P &= -\rho \nabla \phi, \\
\frac{\partial E}{\partial t} + \nabla \cdot [(E + P) \mathbf{v} - \mathbf{B} (\mathbf{B} \mathbf{v})] &= -\rho L, \\
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{vB} - \mathbf{Bv}) &= 0, \\
\nabla^2 \phi &= 4\pi G \rho,
\end{align*}
\]

Post-processing

- Compute the **equilibrium** abundances for all the species (besides \( \text{H}_2 \) and HI)

- Compute the ion-neutral drift velocity \( v_d \)

- Use local physical conditions (\( n, T, A_{\text{V}}, f_{\text{sh,H}_2} \))

<table>
<thead>
<tr>
<th>( \chi )</th>
<th>Mathis 1</th>
<th>mandatory</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_{\text{V}} )</td>
<td>mag 0 – 10</td>
<td>visible extinction</td>
</tr>
<tr>
<td>( T_K )</td>
<td>K 10 – 10(^4)</td>
<td>kinetic temperature</td>
</tr>
<tr>
<td>( n_{\text{H}} )</td>
<td>cm(^{-3}) 10(^{-1}) – 10(^4)</td>
<td>gas density</td>
</tr>
<tr>
<td>( \zeta_{\text{H}_2} )</td>
<td>s(^{-1}) 3 \times 10(^{-16})</td>
<td>CR ionisation rate of ( \text{H}_2 )</td>
</tr>
</tbody>
</table>

| \( f_{\text{sh, H}_2} \) | 10\(^{-8}\) – 1 | \( \text{H}_2 \) self-shielding factor\(^a\) |
| \( f_{\text{sh, CO}} \) | 1 | CO self-shielding factor\(^b\) |
| \( x(\text{H}_2) \) | 10\(^{-2}\) – 1 | \( \text{H}_2 \) abundance |
| \( v_d \) | km s\(^{-1}\) 0 – 5 | ion-neutral velocity drift |

\(^a\) Valdivia et al. (2016) \(^b\) not computed in the simulation
Hybrid Approach For The Chemistry: Validity

Timescales required to reach the equilibrium abundance.

Mass distribution in the simulation 2D PDF: \( f_{sh,H_2} \) vs density

\[ t(H_2) > t_{\text{species}} \quad \& \quad dt > t_{\text{species}} \]

\[ n > 3 \text{ cm}^{-3} \text{ or } f_{sh,H_2} < 10^{-2} \]
This shows that clump histories, that is to say, their ages and the value of the dispersion becomes very high for the less massive clumps, the spatial variations. The bottom panel of Fig. 8. while to investigate the spatial fluctuations at a given time. In As a complement to the time evolution of 4.2.4. Spatial fluctuations for second density bin at time 20 Myr (fourth column, second line) enrichment from the denser gas. This might possibly occur for the three denser density bins) may be compensated for by an en-

That is to say, the time delay to form $H_2$ is close to 1 and the dispersion remains weak. In contrast, $f(H_2)$ is very likely a consequence of turbulent mixing. Because of the low density contained in this low-density bin, this remains a limited distribution dominates the equilibrium distribution. This is most consistent with the fact that the $H_2$ formation does not become fully molecular. This interpretation is also con-

Between 1 and 10 cm$^{-3}$, is slightly puzzling. No significant di-

The second density bin (line 2), which corresponds to a density of a few 100 cm$^{-3}$, could contribute to enhance the more di-

The shielding provided by molecules in gas denser than this value could contribute to enhance the more di-

The local UV flux in which they grow, have a major influence on the formation per density bin (the density increases from purple to red), in the top panel, no threshold is applied. In the middle and bottom panels a threshold of 1000 cm$^{-3}$, respectively, is applied. For the threshold 1000 cm$^{-3}$, the values of $f(H_2)$ decrease by a factor of about 3 for all den-

The difference between the equilibrium and time-dependent distributions becomes eventually less important. For example, the two distributions are obviously close at a time of 20 Myr (right panels) than at a time of 5 Myr.

However, they are not identical. Since all distributions at a time of 15 Myr and 20 Myr are similar, the persistence of the di-

References between the two distributions, which is surprising.

$T \in (316, 1000)$ K

$T \in (1000, 3000)$ K

(Valdivia et al. 2016)
### Compute equilibrium abundances

\( (n, T, A_v, f_{\text{sh}, \text{H}_2}, B) \)

#### Out-of-equilibrium \( \text{H}_2 \):

Non-equilibrium \( \text{H}_2 \) from simulation

#### H\(_2\) at equilibrium:

Abundances at equilibrium for all the species including \( \text{H}_2 \) and \( \text{H}_1 \)

\( (n, T, \text{and shielding from simulation}) \)

---

#### With ion-neutral drift:

Non-equilibrium \( \text{H}_2 \)

Iterative method

- \( \nu_d \approx \frac{\nabla \times B \times B}{4\pi \sum_{jk} n_j n_k \mu_{jk} K_{jk}} \)
- \( T_{\text{eff}} = T_{\text{gas}} + \Delta T \)
- \( \Delta T = \frac{\mu}{3k} \nu_d^2 \)
- \( k \alpha \exp(-\max\{\frac{\beta}{T_{\text{eff}}}, (\beta - 3\Delta T)/T\}) \)

#### Without ion-neutral drift:

Non-equilibrium \( \text{H}_2 \)

- \( \nu_d = 0 \)
- \( T_{\text{gas}} \)
3.2. Role of the ion-neutral drift

The relative velocity between ions and neutrals adds a non-thermal component to the gas temperature, that increases the effective temperature at which ion-neutral reactions occur. To assess the role of the ambipolar diffusion on the production of CH$^+$ we first analyse the distribution of ion-neutral drift velocities and then its impact on the effective temperature distributions.

Figure 2 shows the two-dimensional (2D) probability density functions (PDF) in the form of a 2D histogram of the gas volume, the H$_2$ mass ($m$(H$_2$)), and the CH$^+$ mass ($m$(CH$^+$)) distributions in the simulation box. The left-hand side and central panels show that a large number of cells are characterised by low densities of H$_2$, while a reduced number of cells concentrate most of the mass in H$_2$ form. The right-hand side panel shows that in spite of this distribution, most of the CH$^+$ is produced in regions with intermediate H$_2$ fractions ($f$(H$_2$) $\approx$ 0.3-30%), that do not correspond to the regions which dominate the volume nor the mass of H$_2$, and gas temperatures as high as several $10^2$-$10^3$ K.

We present a single line of sight on Fig. 3 to shed some light on the physical conditions that give rise to an enhancement on the CH$^+$ abundance. This figure shows the local physical condition of the gas, as well as a comparison of the H$_2$ density calculated dynamically in our simulation and what is expected at equilibrium for the same physical conditions (total density, temperature, dust shielding and H$_2$ selfshielding). The bottom panel of this figure shows that most of the CH$^+$ is produced in regions that present specific characteristics favorable to CH$^+$ formation: the fraction of H$_2$ is higher than what is predicted at equilibrium, and temperatures are on the order of several 100 K. In both cases most of the CH$^+$ is produced near the edge of the clumps, but the abundance of CH$^+$ is up to three orders of magnitude larger when the warm H$_2$ is used.

The resulting column densities for the grid of 1024 lines-of-sight are shown in Fig. 4. The column densities of CH$^+$ are 3-10 times higher than those obtained with H$_2$ at equilibrium and closer to the observed ones. However, the abundances are still underpredicted by a factor of $\approx$ 6. This means that the warm H$_2$ plays an important role on the production of CH$^+$, although it is not enough to explain the observed abundances.
Role Of Warm H$_2$: LOS Analysis

![Graph showing the analysis ofWarm H$_2$](image)
Role Of Warm $H_2$: $N(CH^+)$ vs $N_{tot}$
$T_{\text{eff}} = T_{\text{gas}} + \Delta T$  

Residual  

$T_{\text{eff}} = T_{\text{gas}} + \Delta T$  

Residual
Role Of The Ion-Neutral Drift: LOS Analysis

- $n_{tot}$
- $f(H_2)$
- $v_d$
- $T_{eff}$
- $T_{gas}$
- $\log n(CH^+)$
Role Of The Ion-Neutral Drift: \( N(\text{CH}^+) \) vs \( N_{\text{tot}} \)

\[ \mathcal{P}(\log v_d) \propto a, \]

\[ v_d \propto \frac{1}{\rho_i \rho_n} \]
Role Of The Ion-Neutral Drift: LOS Analysis
Summary

- It is possible to make a **hybrid approach** to include the **dynamical effects** on the most sensitive species (those with long evolution times) at a reasonable computational cost: species that react fast can be calculated at equilibrium with respect to the «dynamically» calculated species.

- **Warm H₂** is crucial to efficiently form CH⁺, nevertheless the abundances of CH⁺ are still **underpredicted** compared to observations (Crane et al. 1995; Gredel 1997; Weselak et al. 2008)

- The formation of CH⁺ seems to be more efficient in **regions where H₂ is not expected at equilibrium**.

- **High ion-neutral drift velocities** can boost the CH⁺ formation, but these events are extremely rare => The effect is **negligible**.

- A good description of **small-scale physics** is necessary to avoid unrealistic $v_d$ distributions.

- **Possible clues:** dissipation of turbulence (Falgarone et al. 2010, Godard et al. 2009, 2014), UV pumped H₂ levels (Zanchet et al. 2013; Herráez-Aguilar et al. 2014)
Ideal MHD multiphase simulation

RAMSES AMR code
(Teyssier 2002)

\( L = 50 \) pc
\( N = 1 \) cm\(^{-3}\)
\( V_{\text{in}} = 15 \) km s\(^{-1}\)
\( B = 2.5 \) \( \mu \)G
\( dx_{\text{min}} = 0.05 \) pc
\( dx_{\text{max}} = 0.2 \) pc

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \]
\[ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} - \mathbf{B} \mathbf{B}) + \nabla P = -\rho \nabla \phi, \]
\[ \frac{\partial E}{\partial t} + \nabla \cdot [(E + P) \mathbf{v} - \mathbf{B} (\mathbf{B} \mathbf{v})] = -\rho \mathcal{L}, \]
\[ \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v}) = 0, \]
\[ \nabla^2 \phi = 4\pi G \rho, \]

(Valdivia et al. 2016)

\[ \frac{\partial n_{\text{H}_2}}{\partial t} + \nabla \cdot (n_{\text{H}_2} \mathbf{v}) = k_{\text{form}} n (n - 2n_{\text{H}_2}) - k_{\text{ph}} n_{\text{H}_2}. \]
Clumps are dominated by the turbulent pressure => Transient structures

\( 
\text{H}_2 \text{ can be transported from cold and dense regions towards warm and diluted environments, where it survives due to the shielding provided by the multiphase structure} 
\)
H$_2$ formation on grain surfaces

H$_2$ formation interpreted as an extinction of starlight due to the presence of small solid particles, or fine cosmic dust. Now we know that dust represents only about 1% of the total mass of the ISM, but it plays a key role in astrophysical contexts. It shields the gas against UV radiation, and acts as a catalyst for several reactions, H$_2$ formation being the most relevant (Gould and Salpeter 1963; Hollenbach and Salpeter 1971).

H$_2$ can be formed on grain surfaces in two pathways: the Eley-Rideal (ER) mechanism and the Langmuir-Hinshelwood (LH) mechanism. Fig. 2.4 shows the two mechanisms. A detailed study of H$_2$ formation on dust grains, paying particular attention to these two pathways to form molecular hydrogen, has been recently performed by Bron (2014) in his thesis work.

Figure 2.4: Two main paths for the formation of molecular hydrogen on grain surface: (a) shows the Eley-Rideal mechanism, while (b) shows the Langmuir-Hinshelwood mechanism.

In the case of ER mechanism, a chemisorbed atom reacts with a gas-phase hydrogen atom. The adsorbed atom is chemically bonded to the grain surface, and it is not able to move. The second atom, still in gas-phase, hits the adsorbed atom to form an H$_2$ molecule, liberating some $4.5 \ eV$. A part of the released energy is used to desorb the molecule.

The LH mechanism differs in the nature of the bond between hydrogen atoms and the grain surface. In this case the atom is physisorbed, and the bond is much weaker. This allows the molecule to wander over the grain surface until it encounters another adsorbed atom to form a new molecule. As in the ER mechanism, the molecule is desorbed by using part of the energy released by the reaction.

These mechanisms are essentially different from the mechanisms operating in gas-phase. In the case of H$_2$ formation on grain surfaces the excess energy is evacuated in a non-radiative manner.

Estimate of H$_2$ formation rate

The formation rate of H$_2$ can be estimated using the collision rate between hydrogen atoms and grains, considering that two collisions are needed to form one molecule. This can be written in the following manner:

$$\frac{dn}{dt} \approx \frac{1}{2} n(HI) n_{gr} \Sigma_{gr} v_{th} \ (2.15)$$

$$k_{\text{form}} = 3 \times 10^{-17} \times \sqrt{\frac{T}{100 \ K}} \times \frac{1}{1 + \left(\frac{T}{464 \ K}\right)^{1.5}} \ \text{cm}^3\text{s}^{-1}$$

$k_0$ (Jura 1974)

Sticking factor (Le Bourlot et al. 2012, Bron et al. 2014)
H$_2$ destruction by UV fluorescent photodissociation

\[ k_{ph} = 3.3 \times 10^{-11} \times G_0 < e^{-\sigma_d N} \times f_{\text{shield}}(N_{H_2}) > \text{s}^{-1} \]

- Dust shielding
- Self-shielding (Draine & Bertoldi 1996)

Tree-based method (Valdivia & Hennebelle, 2014)
**Cooling:**

- **H₂ line emission:** (Le Bourlot et al. 1999)

\[
W(H_2) = \frac{1}{n(H_2)} \sum_{vJ,v'J'} (E_{vJ} - E_{v'J'}) n_{vJ} A(vJ \rightarrow v'J')
\]

**Heating:**

- **H₂ formation:** 1.5 eV
- **H₂ destruction:** 0.4 eV (Black & Dalgarno 1977, Glover & Mac Low 2007)