Origin Of CH^+ In Diffuse Molecular Clouds

Outline

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(A&A in press)

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CH⁺ in the diffuse ISM

- Simple hydride

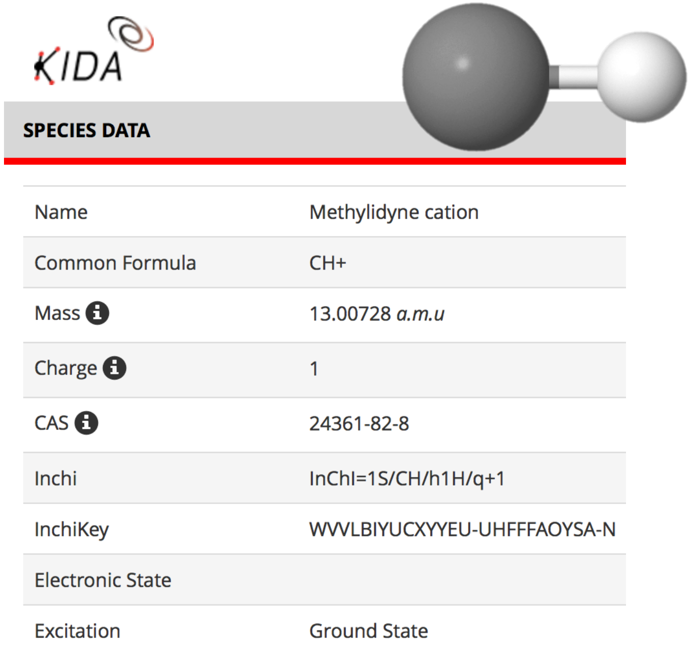
- Easily **destroyed**

- Main formation path is **highly endothermic**

$$C^+ + \underbrace{H_2}_{} \rightarrow CH^+ + H \qquad (\Delta E/k = \underbrace{-4300\ K}_{}).$$

- Classical PDR models **predict low abundances** in the diffuse ISM

- But observations reveal **relatively high abundances**



KIDA

SPECIES DATA

Name	Methylidyne cation
Common Formula	CH+
Mass	13.00728 *a.m.u*
Charge	1
CAS	24361-82-8
Inchi	InChI=1S/CH/h1H/q+1
InchiKey	WVVLBIYUCXYYEU-UHFFFAOYSA-N
Electronic State	
Excitation	Ground State

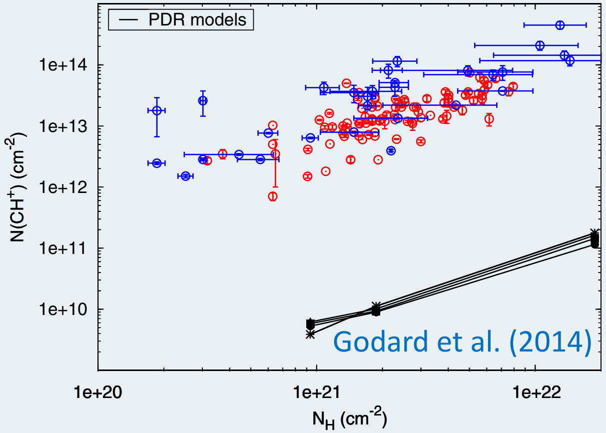
CH^+ In The Diffuse ISM: Goal

Impact of the turbulent mixing CNM/WNM on the chemistry
Impact of the multiphase structure

CH^+ In The Diffuse ISM: Previous Attempts

PDR Models

Stationary plane-parallel slabs illuminated from one or two sides



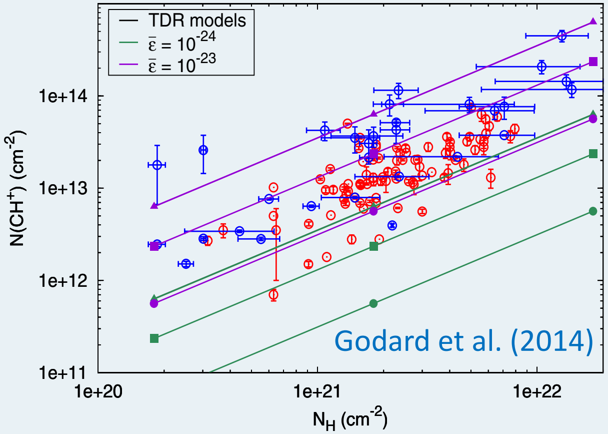
Godard et al. (2014)

Simple geometry, it does not take into account the dynamics nor the fractal-like structure of real molecular clouds.

Dissipation of Turbulence

Burst of dissipation

L~10 AU ; t~100 yr



Godard et al. (2014)

Do not consider the role of gas dynamics nor the 3D structure

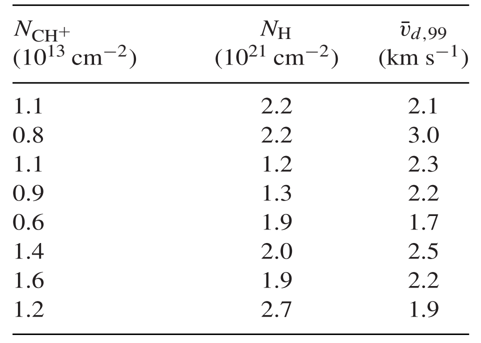
Underlying dissipation processes are imposed

(Falgarone et al. 2010, Godard et al. 2009, 2014)

Ion-Neutral Drift

$$T_{\rm eff} = \frac{m_i T_n + m_n T_i}{m_i + m_n} + \Delta T$$

$$\Delta T = \frac{\mu}{3k} v_{\rm d}^2$$



$N_{\rm CH^+}$ (10^{13} cm^{-2})	$N_{\rm H}$ (10^{21} cm^{-2})	$\bar{v}_{d,99}$ (km s^{-1})
1.1	2.2	2.1
0.8	2.2	3.0
1.1	1.2	2.3
0.9	1.3	2.2
0.6	1.9	1.7
1.4	2.0	2.5
1.6	1.9	2.2
1.2	2.7	1.9

Myers et al. (2015)

Do not treat microphysics

Constant ion density

(Myers et al. 2015)

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

Hybrid Approach For The Chemistry

On-the-fly

- Crucial species for the chemistry: **H_2** which is a **bottleneck** for the chemistry.

$$\frac{\partial n_{\mathrm{H_2}}}{\partial t} + \nabla \cdot (n_{\mathrm{H_2}} \boldsymbol{v}) = k_{\mathrm{form}} n (n - 2n_{\mathrm{H_2}}) - k_{\mathrm{ph}} n_{\mathrm{H_2}}$$

- Heating: PE, CR, H_2 (formation and destruction)
- Use cooling functions: CII, OI, Lyα, Rec, H_2
- Compute dust shielding and H_2 self-shielding $f_{\mathrm{sh,\,H2}} = < e^{-\tau_{d,1000}} f_{\mathrm{shield}} >$
- Solve ideal MHD equations.

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

Post-processing

- Compute the **equilibrium** abundances for all the species (besides H_2 and HI)
- Compute the ion-neutral drift velocity v_d
- Use local physical conditions (n, T, Av, $f_{\mathrm{sh,H2}}$)

		mandatory	
χ	Mathis	1	external UV radiation field
A_V	mag	$0 - 10$	visible extinction
T_K	K	$10 - 10^4$	kinetic temperature
n_{H}	$\mathrm{cm^{-3}}$	$10^{-1} - 10^4$	gas density
$\zeta_{\mathrm{H_2}}$	$\mathrm{s^{-1}}$	3×10^{-16}	CR ionisation rate of H_2
		optional	
$f_{\mathrm{sh,\,H_2}}$		$10^{-8} - 1$	H_2 self-shielding factor[a]
$f_{\mathrm{sh,\,CO}}$		1	CO self-shielding factor[b]
$x(\mathrm{H_2})$		$10^{-7} - 1$	H_2 abundance
v_{d}	$\mathrm{km\ s^{-1}}$	$0 - 5$	ion-neutral velocity drift

(*a*) Valdivia et al. (2016) (*b*) not computed in the simulation

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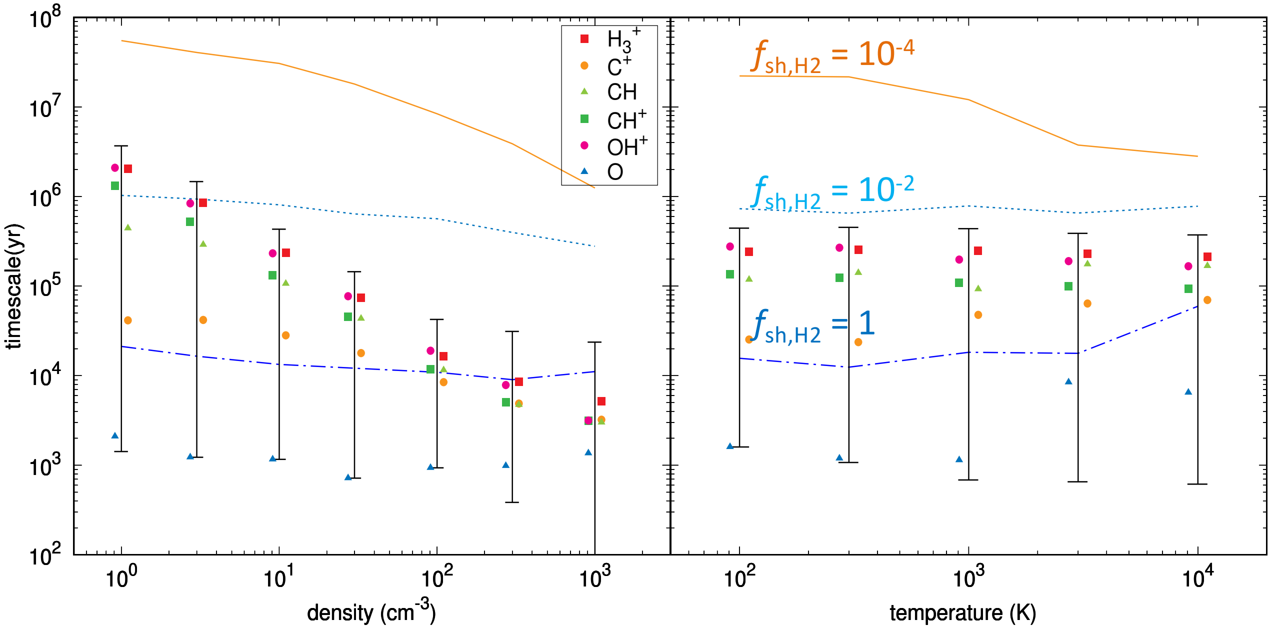
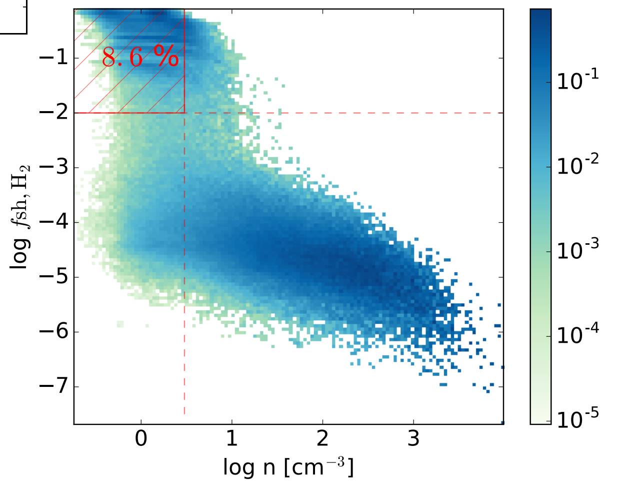
Hybrid Approach For The Chemistry: Validity



Timescales required to reach the equilibrium abundance.

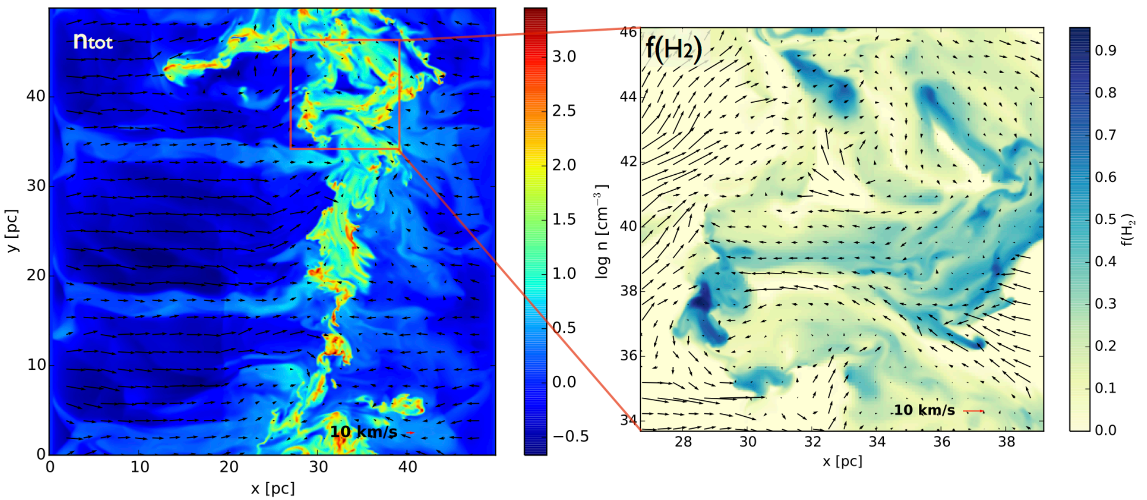
$t(H_2) > t_{species}$ & $dt > t_{species}$

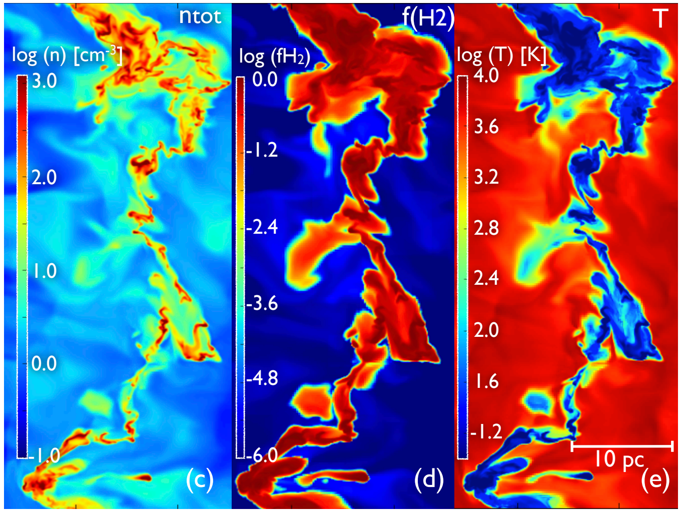
$n > 3\ cm^{-3}$ or $f_{sh,H2} < 10^{-2}$

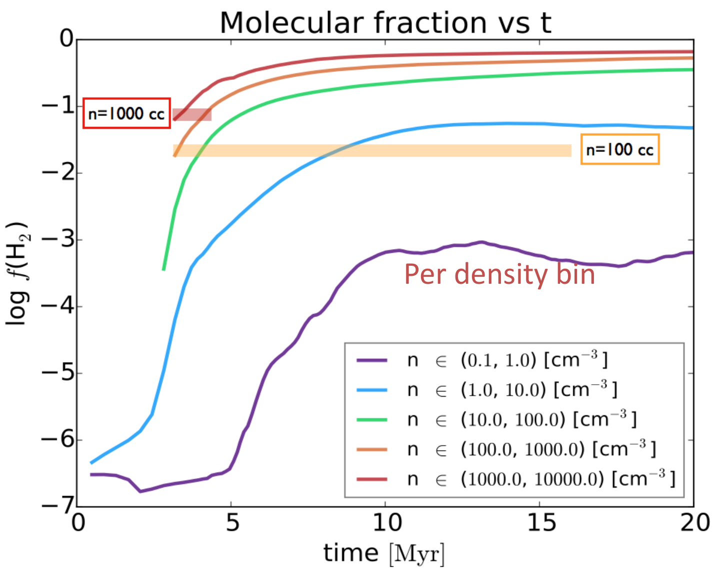


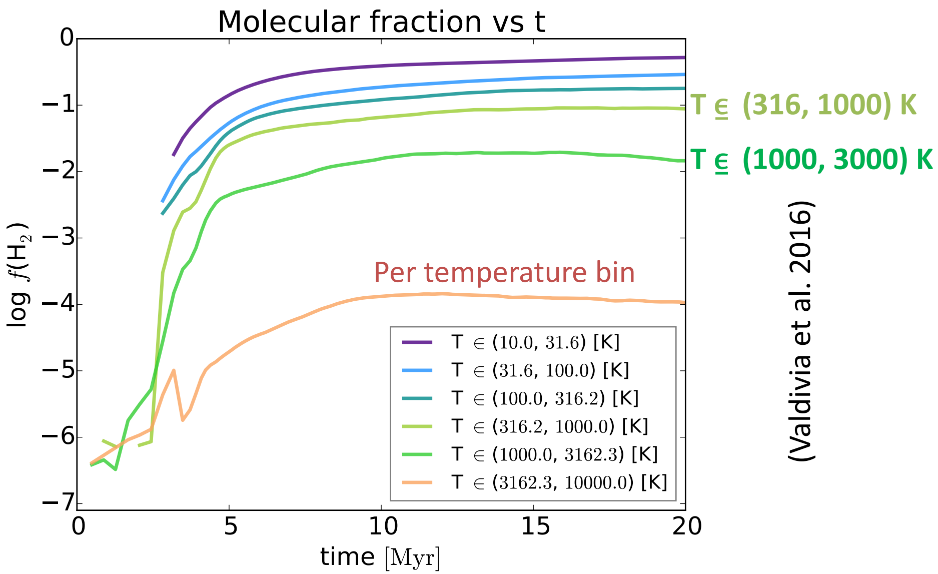
Mass distribution in the simulation
2D PDF: $f_{sh,H2}$ vs density

Numerical Simulation: Results On H_2









(Valdivia et al. 2016)

(Valdivia et al. 2016)

Post-processing:

Compute equilibrium abundances $(n, T, \mathrm{Av}, f_{\mathrm{sh,H2}}, \boldsymbol{B})$

Out-of-equilibrium H_2: Non-equilibrium H_2 from simulation	**H_2 at equilibrium:** Abundances at equilibrium for all the species including H_2 and HI (n, T, and shielding from simulation)
With ion-neutral drift: Non-equilibrium H_2 Iterative method • $v_{\mathrm{d}} \approx \frac{(\nabla\times\boldsymbol{B})\times\boldsymbol{B}}{4\pi\sum_{jk} n_j n_k \mu_{jk} K_{jk}}$ • $T_{\mathrm{eff}} = T_{\mathrm{gas}} + \Delta T$ • $\Delta T = \frac{\mu}{3k} {v_d}^2$ • $k \ \alpha \ \exp(-\max\{\frac{\beta}{T_{\mathrm{eff}}}, (\beta - 3\Delta T)/T\})$	**Without ion-neutral drift:** Non-equilibrium H_2 $v_{\mathrm{d}} = 0$ T_{gas}

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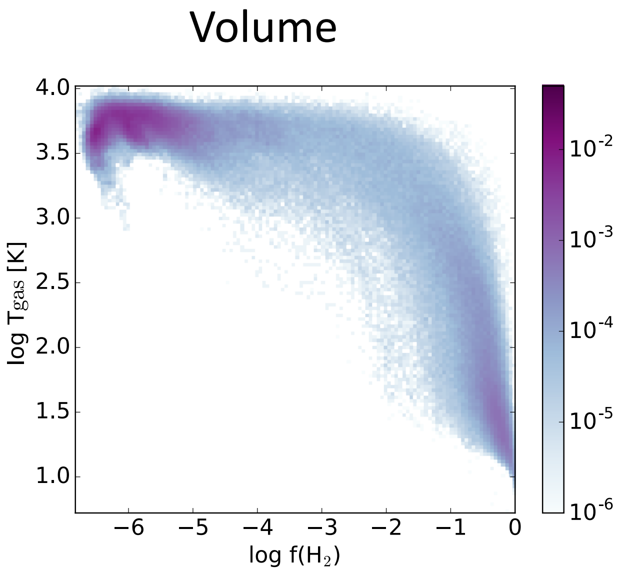
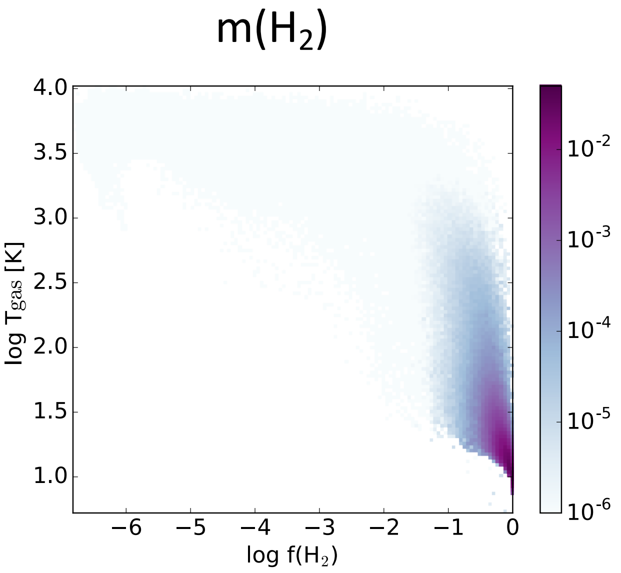
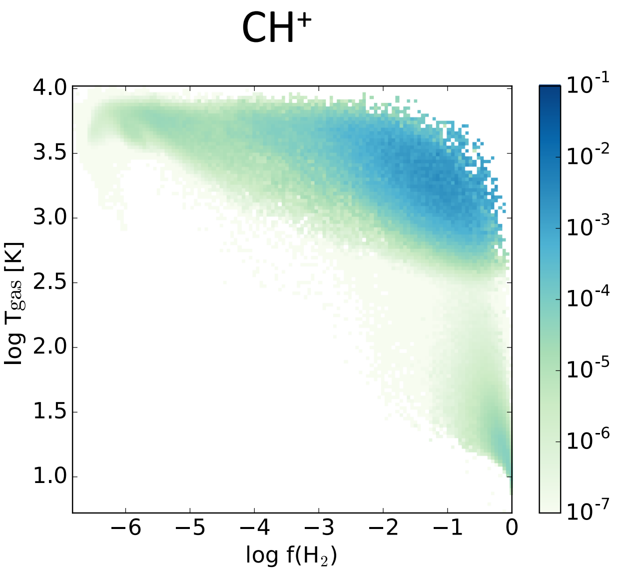
Role Of Warm H_2: 2D PDF


Volume


$m(H_2)$


CH^+

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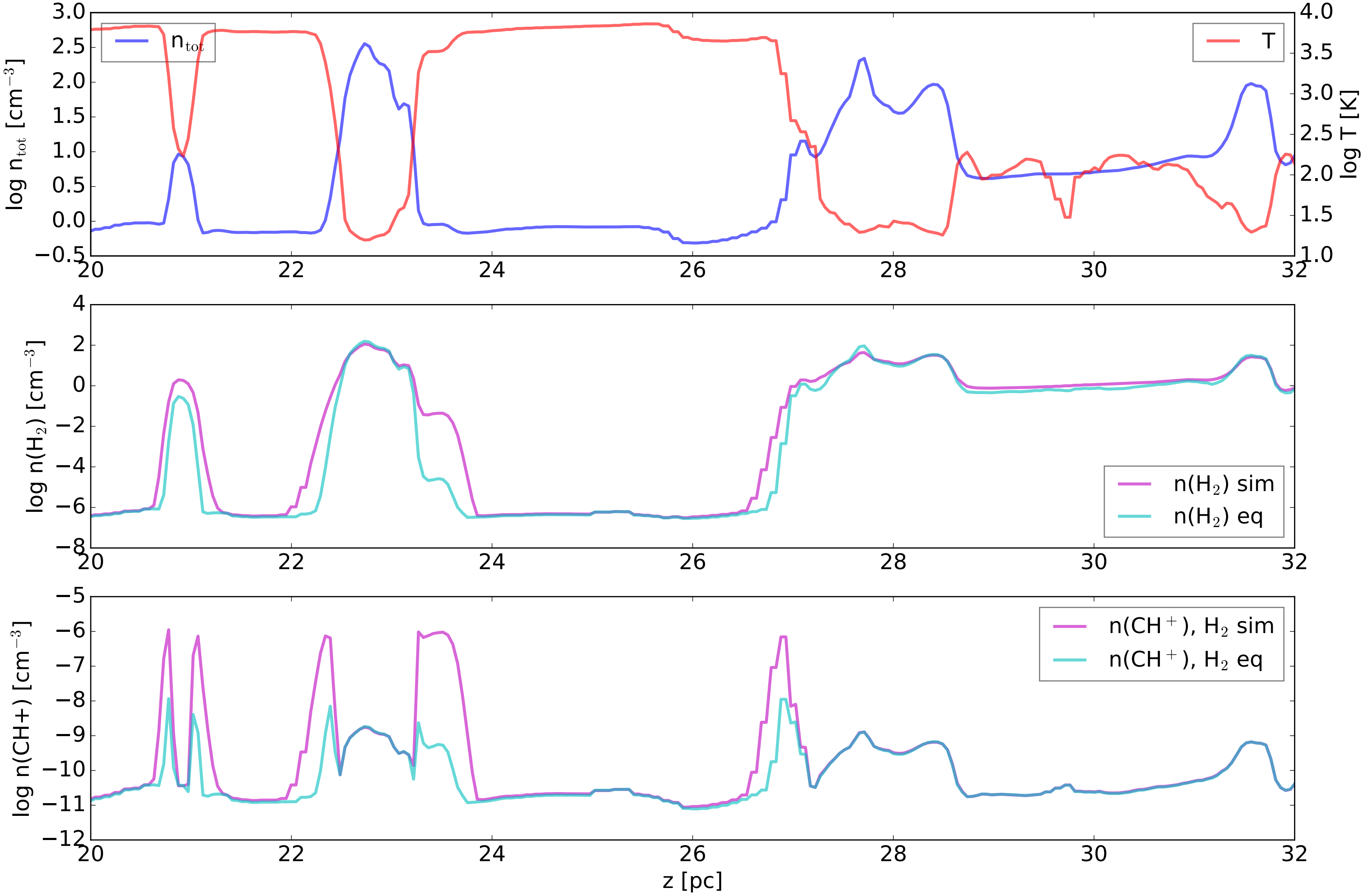
Role Of Warm H_2: LOS Analysis



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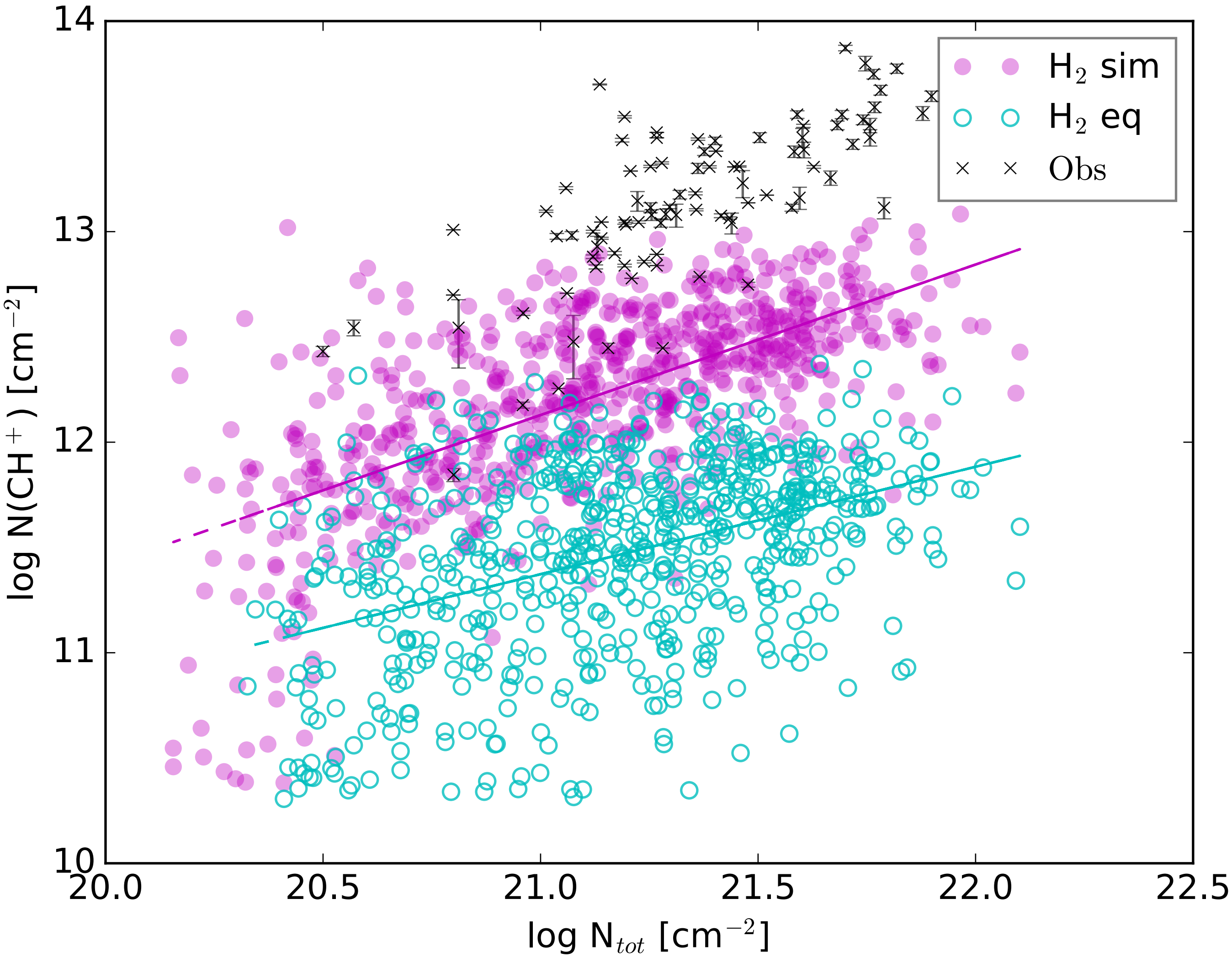
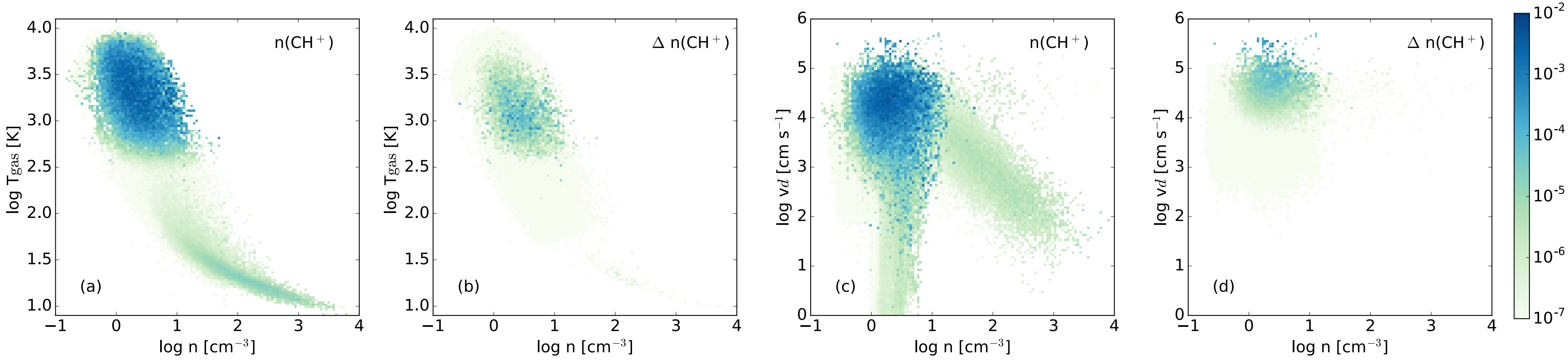
THE HYDRIDE TOOLBOX

Role Of Warm H_2: $N(CH^+)$ vs N_{tot}



Role Of The Ion-Neutral Drift: 2D PDF



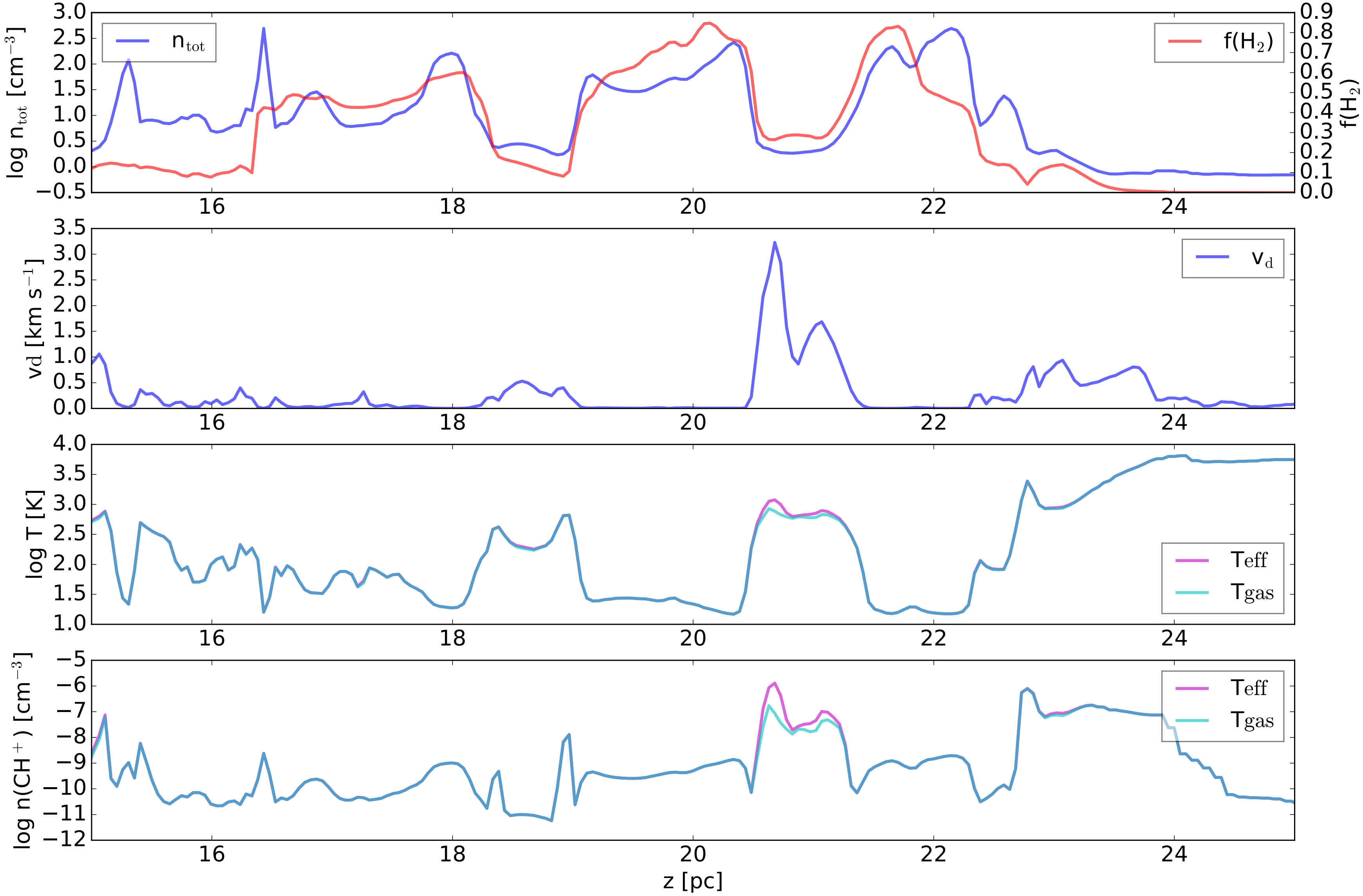
$T_{eff} = T_{gas} + \Delta T$

Residual

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

Residual

Role Of The Ion-Neutral Drift: LOS Analysis



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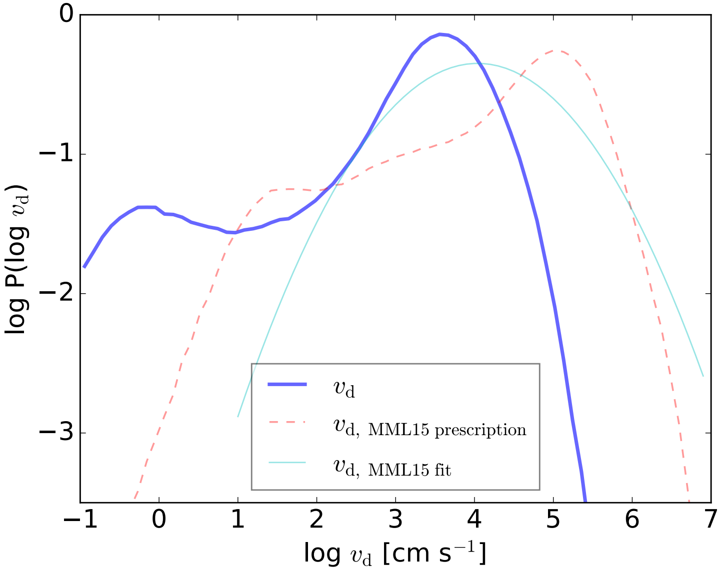
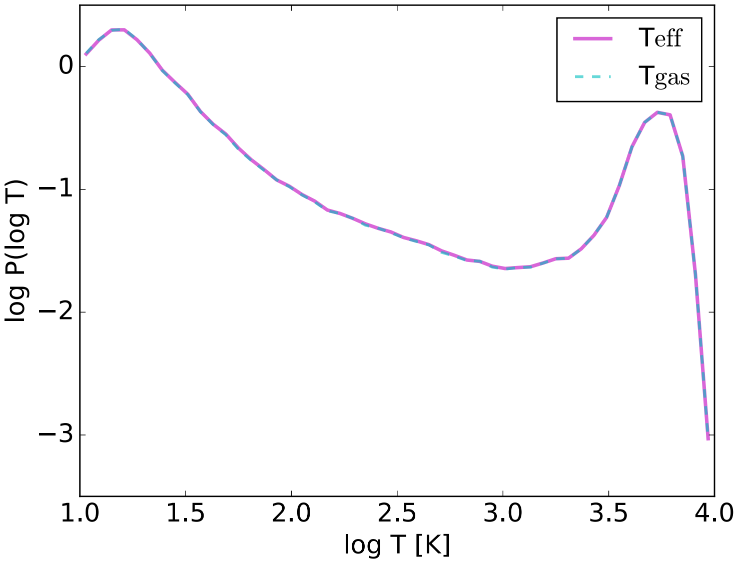
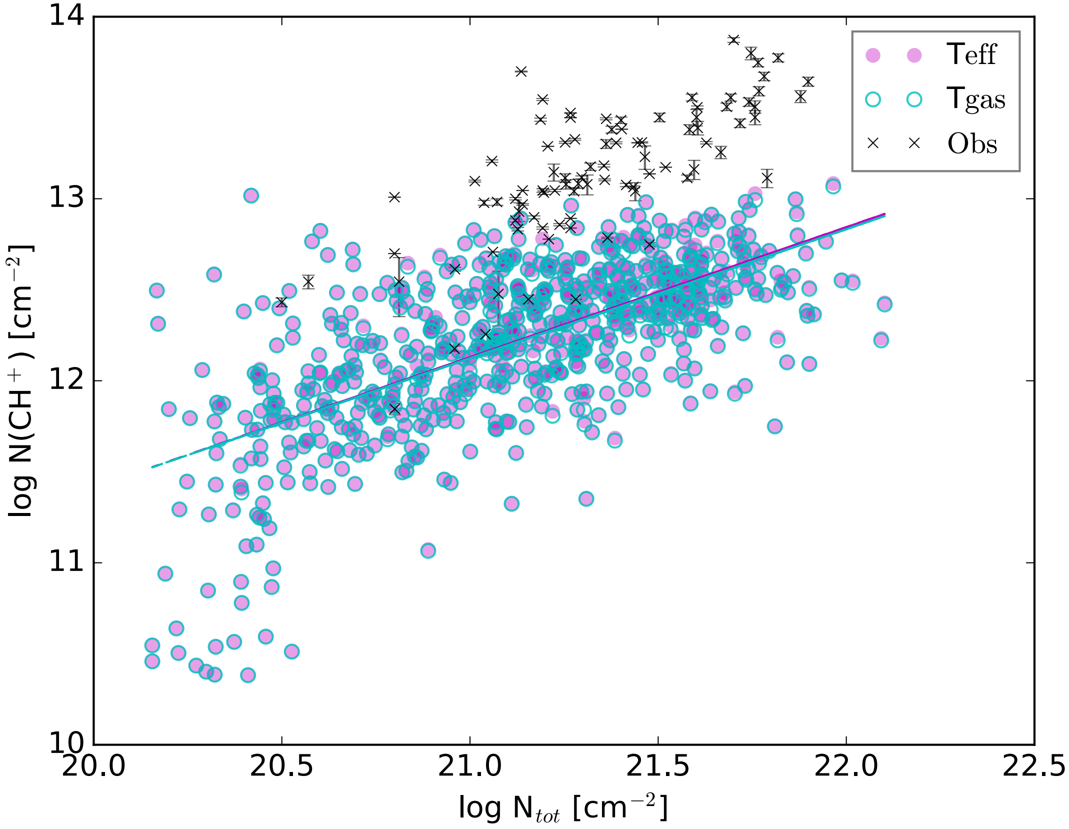
Role Of The Ion-Neutral Drift: N(CH$^+$) vs N$_{tot}$







- $v_\mathrm{d} \propto \frac{1}{\rho_i \rho_n}$

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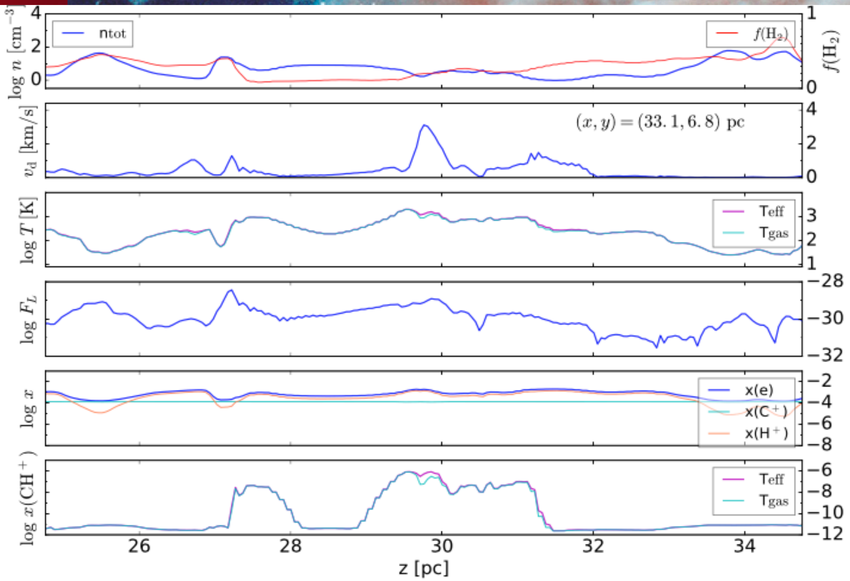
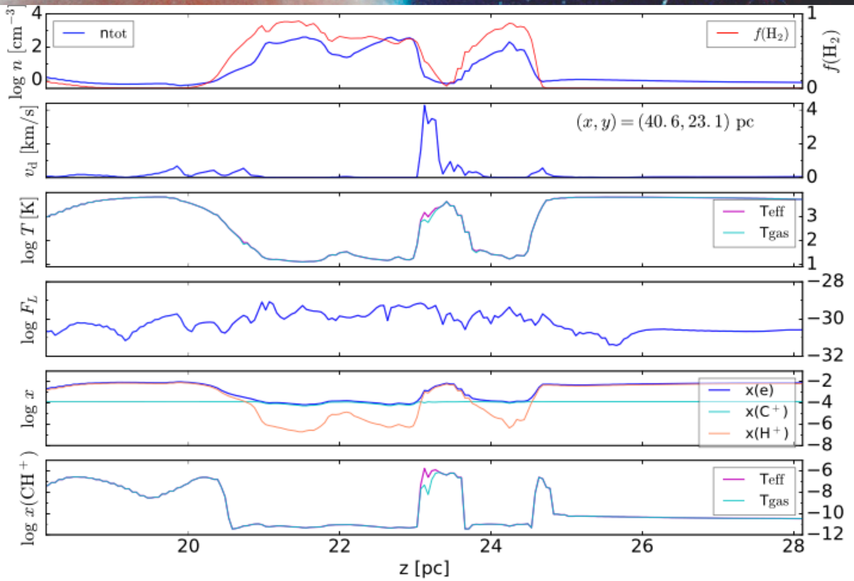
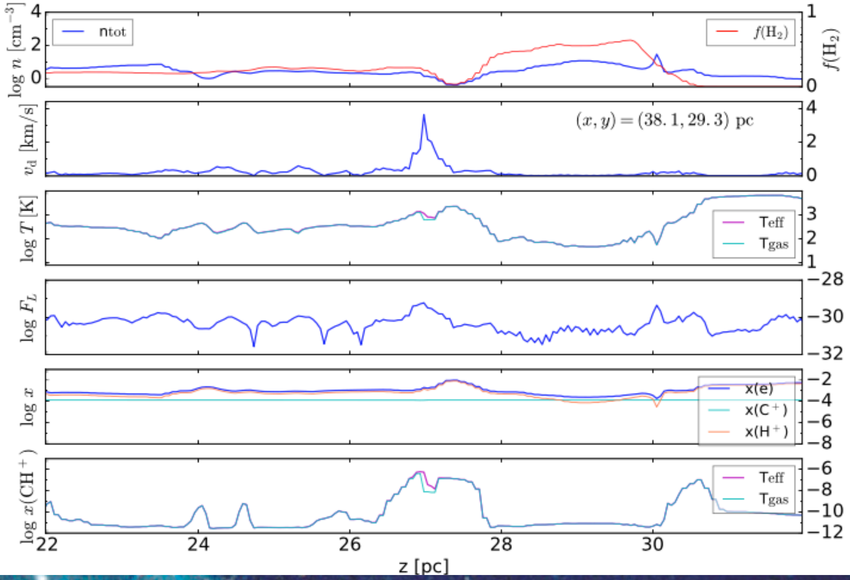
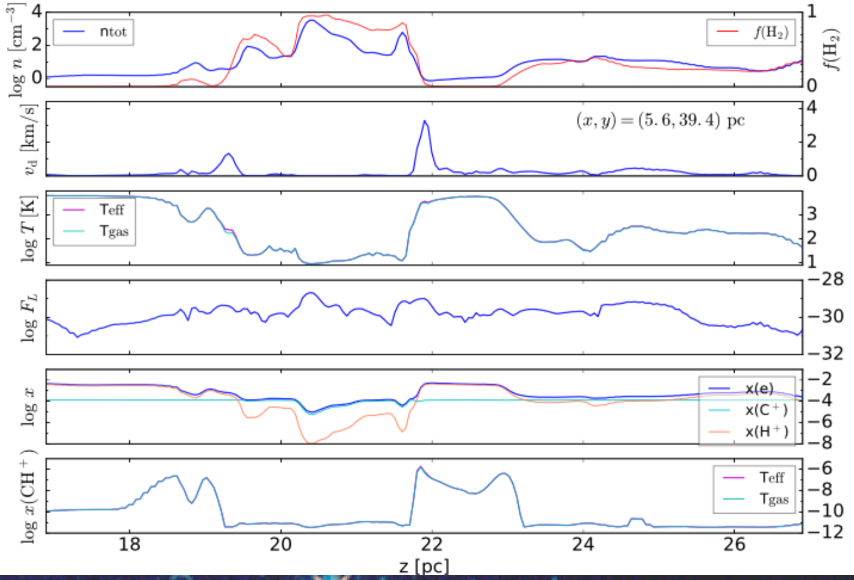
Role Of The Ion-Neutral Drift: LOS Analysis









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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 H_2** 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 H_2 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.

- **<u>Possible clues:</u>** dissipation of turbulence (Falgarone et al. 2010, Godard et al. 2009, 2014), UV pumped H_2 levels (Zanchet et al. 2013; Herráez-Aguilar et al. 2014)

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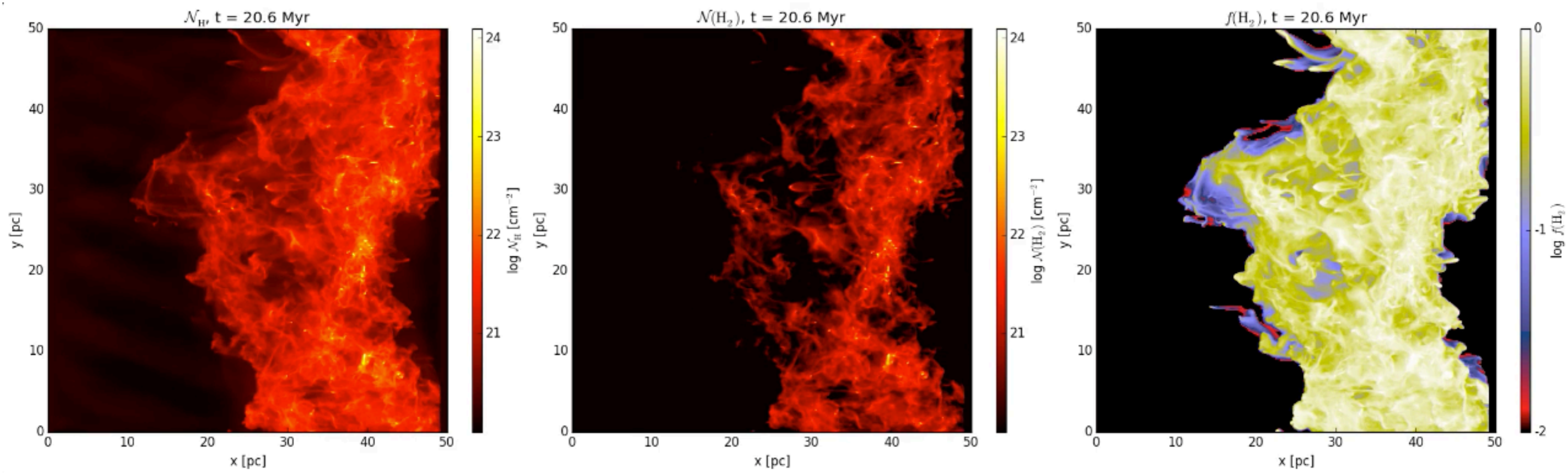
Extra slides

Ideal MHD multiphase simulation



RAMSES AMR code

(Teyssier 2002)

$L = 50$ pc

$N = 1$ cm^{-3}

$V_{in} = 15$ km s^{-1}

$B = 2.5$ μG

$dx_{min} = 0.05$ pc

$dx_{max} = 0.2$ pc

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

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} - \boldsymbol{B}\boldsymbol{B}) + \nabla P = -\rho \nabla \phi,$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + P)\boldsymbol{v} - \boldsymbol{B}(\boldsymbol{B}\boldsymbol{v})] = -\rho \mathcal{L},$$

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

$$\nabla^2 \phi = 4\pi G \rho,$$

(Valdivia et al. 2016)

$$\frac{\partial n_{H_2}}{\partial t} + \nabla \cdot (n_{H_2} \boldsymbol{v}) = k_{form} n(n - 2n_{H_2}) - k_{ph} n_{H_2}$$

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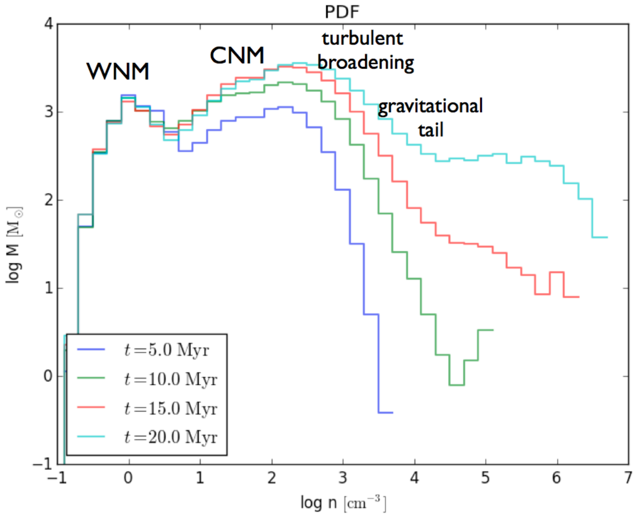
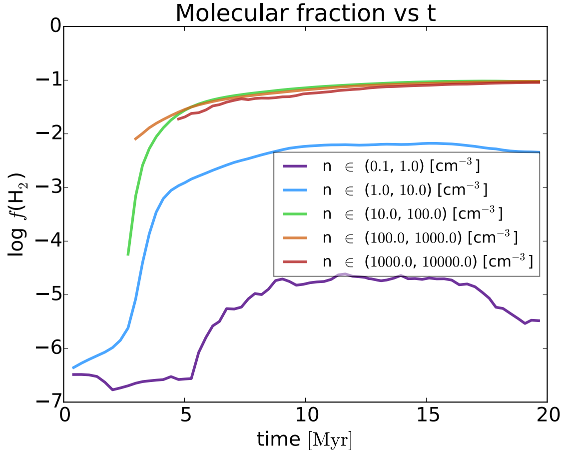
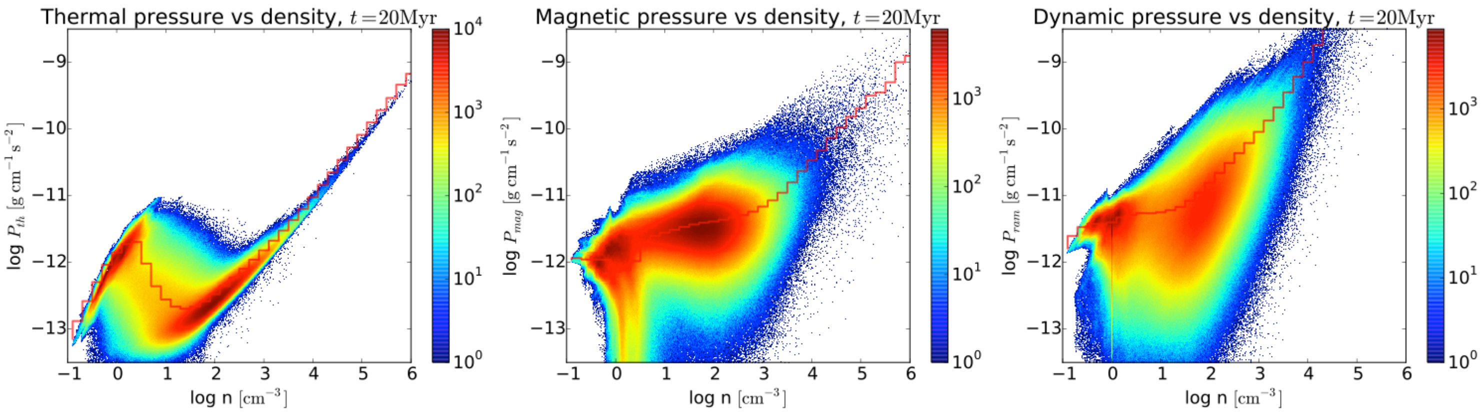
Origin of warm H_2



H_2 formation suppressed for $n_{thresh} \geq 100$ cm^{-3}



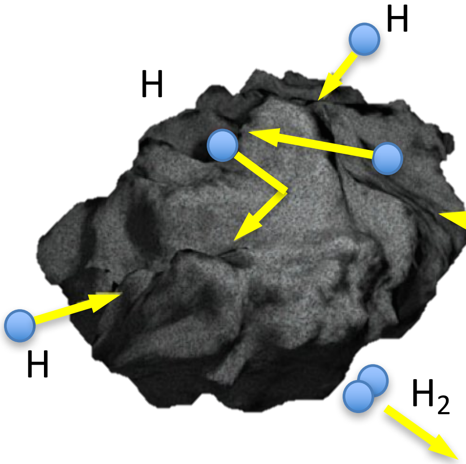
(Valdivia et al. 2016)

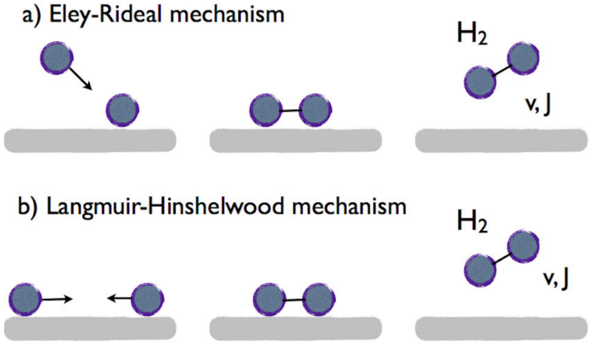


- Clumps are dominated by the **turbulent pressure** => **Transient** structures
- H_2 can be **transported** from cold and dense regions towards **warm and diluted** environments, where it survives due to the shielding provided by the **multiphase structure**

H_2 formation

H_2 formation on grain surfaces





$$k_{\mathrm{form}} = \underbrace{3 \times 10^{-17}}_{k_0\ \text{(Jura 1974)}} \times \sqrt{\frac{T}{100\ \mathrm{K}}} \times \underbrace{\frac{1}{1 + \left(\frac{T}{464\ \mathrm{K}}\right)^{1.5}}}_{\text{Sticking factor (Le Bourlot et al. 2012, Bron et al. 2014)}}\ \mathrm{cm}^3\mathrm{s}^{-1}$$

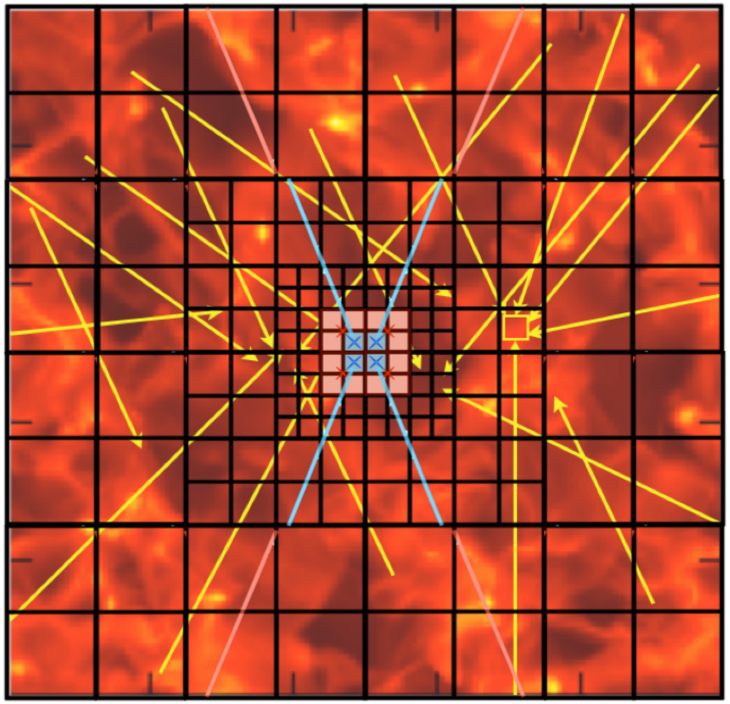
H_2 destruction

H_2 destruction by UV fluorescent photodissociation

$$k_{\mathrm{ph}} = 3.3 \times 10^{-11} \times G_0 < \underbrace{\mathrm{e}^{-\sigma_d \mathcal{N}}}_{\text{Dust shielding}} \times \underbrace{f_{\mathrm{shield}}(\mathcal{N}_{\mathrm{H_2}})}_{\text{Self-shielding}} > \ \mathrm{s}^{-1}$$

(Draine & Bertoldi 1996)

UV photons



Tree-based method (Valdivia & Hennebelle, 2014)

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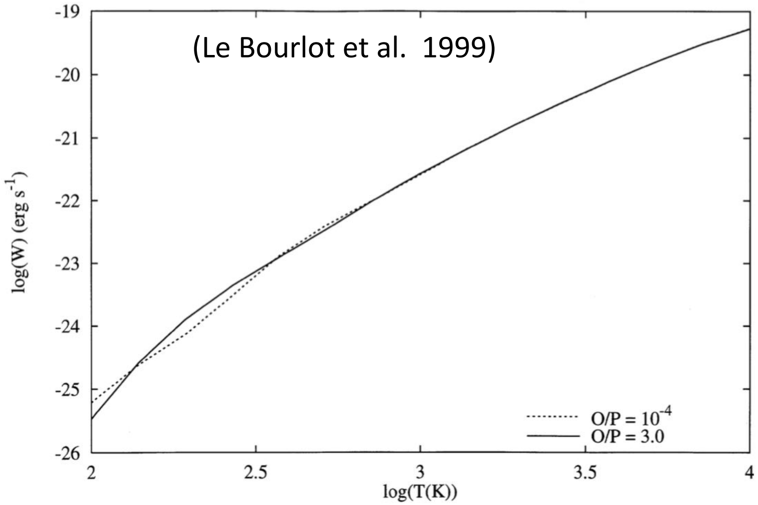
H_2 Thermal feedback

Cooling:

- H_2 line emission: (Le Bourlot et al. 1999)

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



Heating:

- H_2 formation: 1.5 eV
- H_2 destruction: 0.4 eV (Black & Dalgarno 1977, Glover & Mac Low 2007)

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