Physical and chemical evolution from diffuse to dense clouds

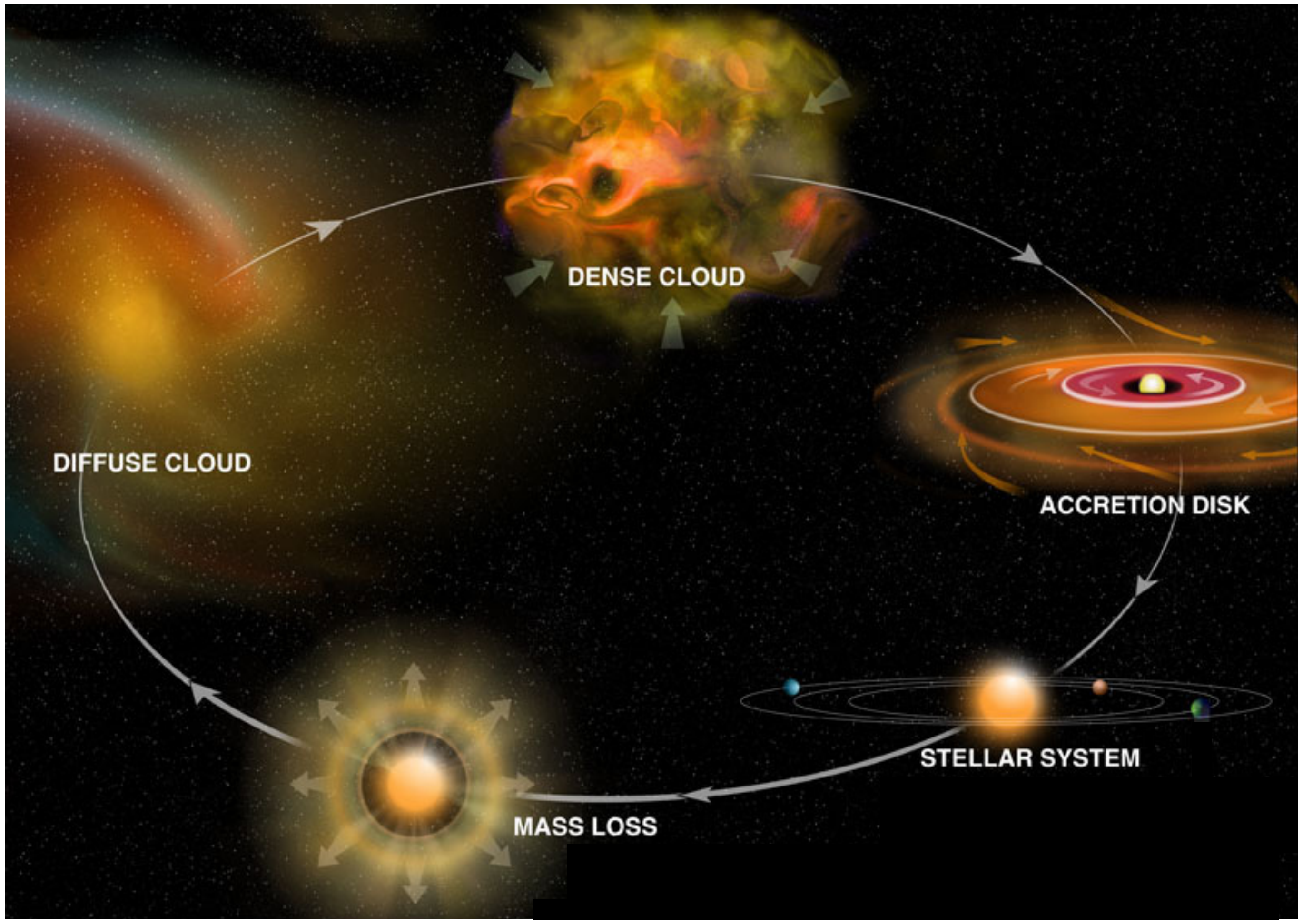
Maxime Ruaud
NPP Fellow at NASA Ames

Introduction

Physical and chemical evolution are intimately linked

- Atoms and molecules provide the cooling
  - Ly-α HI
  - Fine structure lines: [C II], [O I],…
  - Rotational lines: H_2, CO, OH, H_2O…

- Molecular observations give insight on the physics

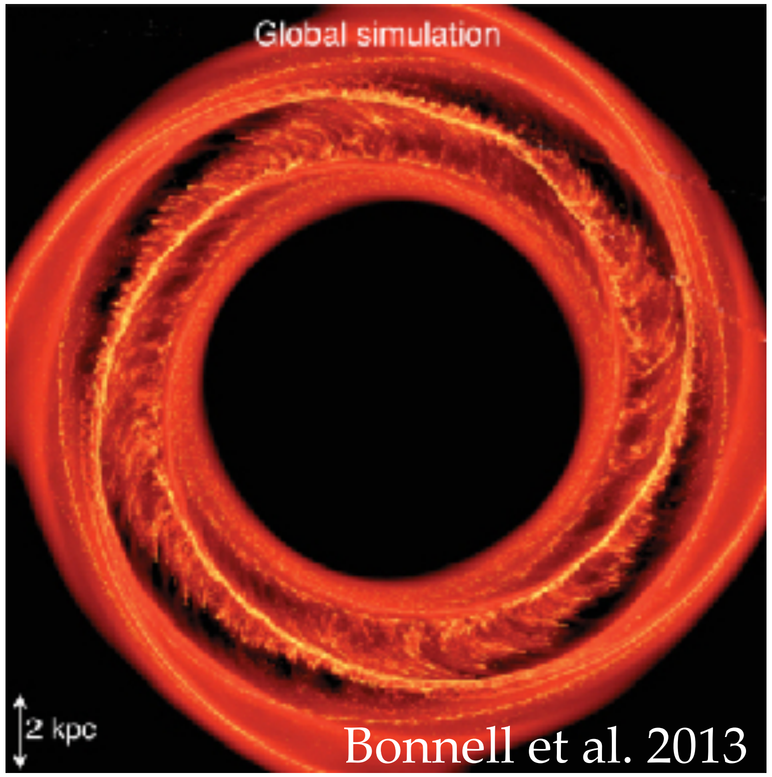


Introduction

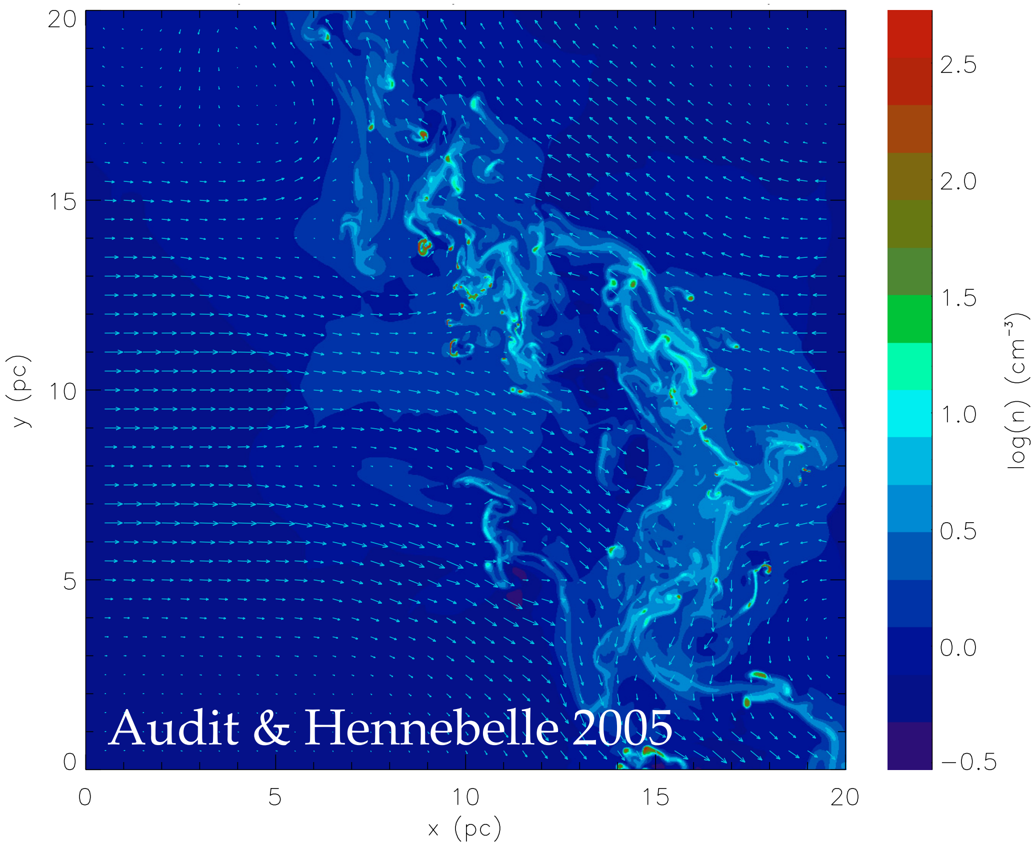
Dynamical evolution

Both large scale and small scale MHD simulations reach approximately same conclusion:

- Atomic and molecular clouds form by converging flows of the WNM
  - Produce a turbulent shocked thermal unstable layer which fragments
  - Turbulence maintained by interaction with the WNM
- Gravity takes over when enough gas has accumulated



Bonnell et al. 2013



Audit & Hennebelle 2005

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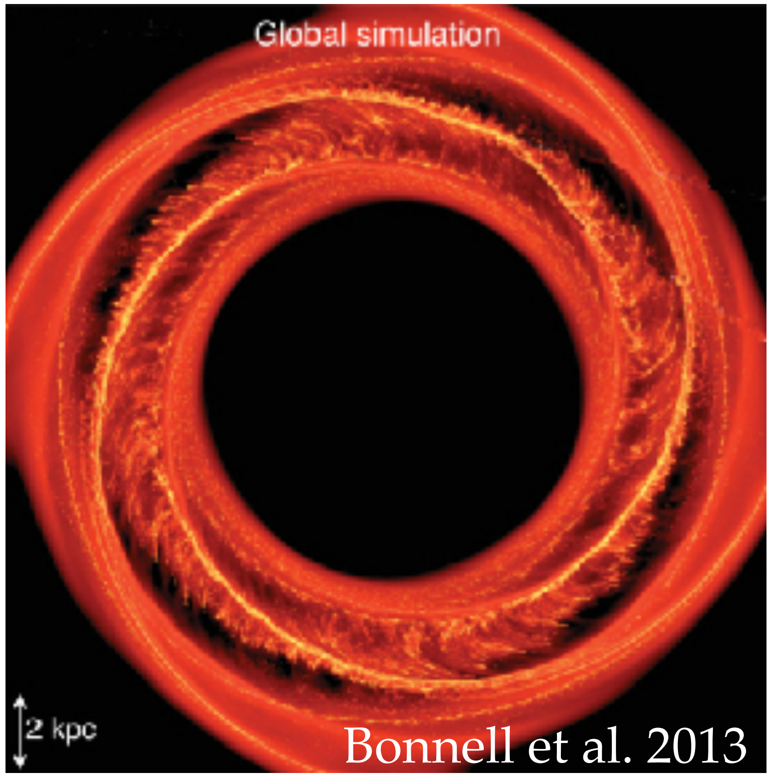
Interstellar clouds are continuously evolving objects and strongly coupled to their environment



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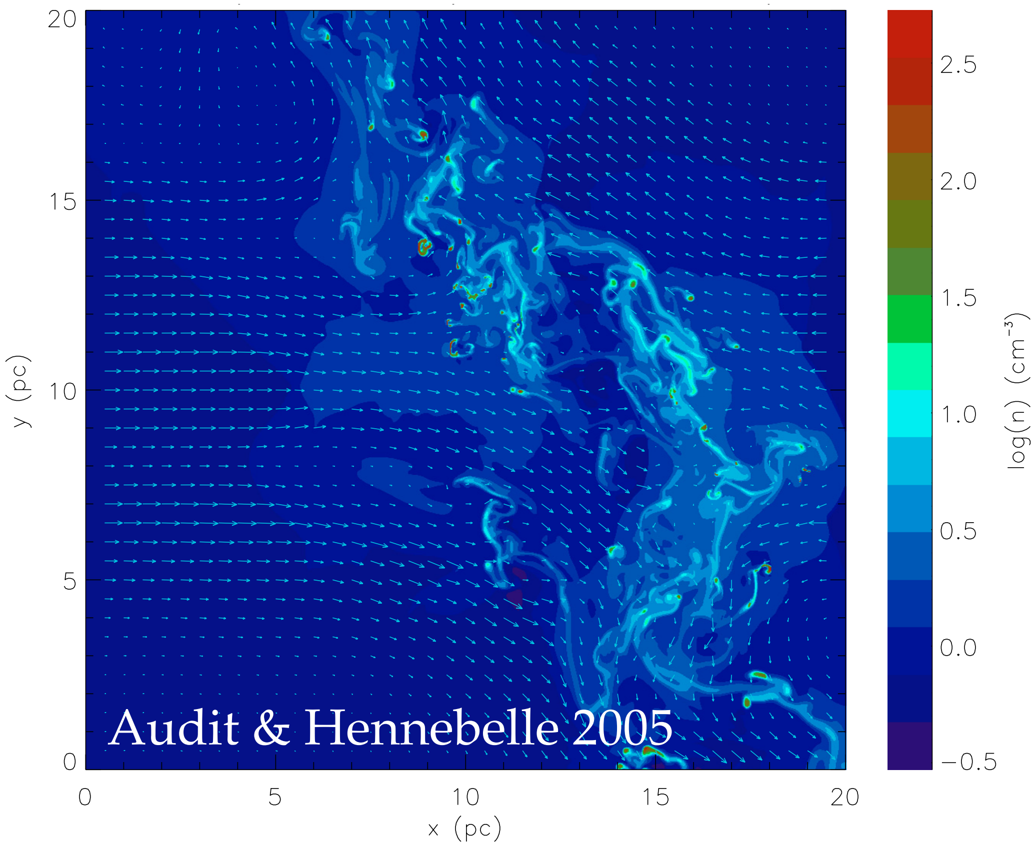
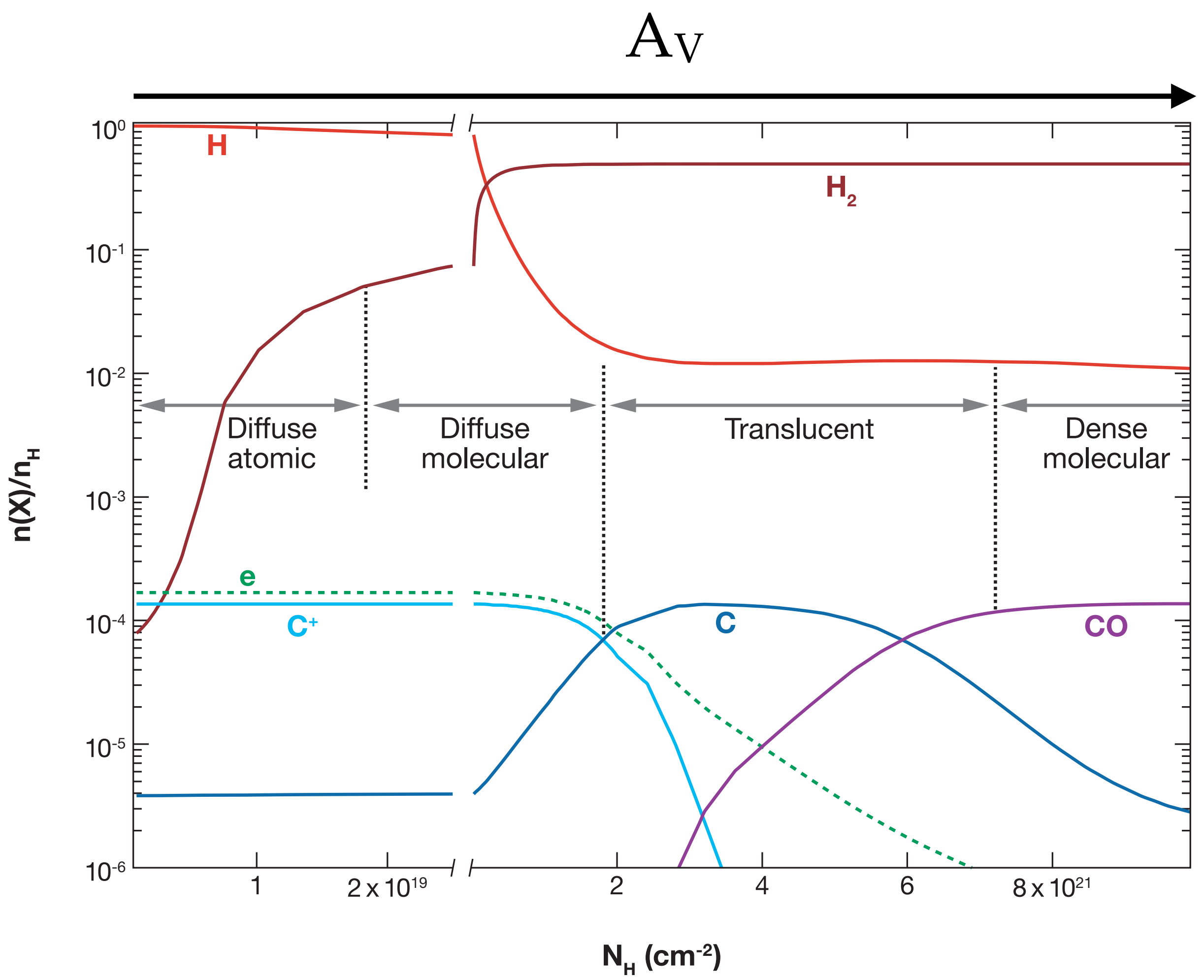


Audit & Hennebelle 2005

Introduction

	Diffuse Atomic	Diffuse Molecular	Translucent	Dense Molecular
Defining Characteristic	$f^n{}_{H_2} < 0.1$	$f^n{}_{H_2} > 0.1$ $f^n{}_{C+} > 0.5$	$f^n{}_{C+} < 0.5$ $f^n{}_{CO} < 0.9$	$f^n{}_{CO} > 0.9$
A_V (min.)	0	~0.2	~1–2	~5–10
Typ. n_H (cm^{-3})	10–100	100–500	500–5000?	$>10^4$
Typ. T (K)	30–100	30–100	15–50?	10–50
Observational Techniques	UV/Vis H I 21-cm	UV/Vis IR abs mm abs	Vis (UV?) IR abs mm abs/em	IR abs mm em

Snow and Mc Call 2006



Molecular fraction

$$f(\mathrm{H_2}) = \frac{2N(\mathrm{H_2})}{N(\mathrm{H}) + 2N(\mathrm{H_2})}$$

Visual extinction

$$A_V \sim 5.8 \times 10^{-22} \left(\frac{N_\mathrm{H}}{1\ \mathrm{cm}^{-2}} \right)$$

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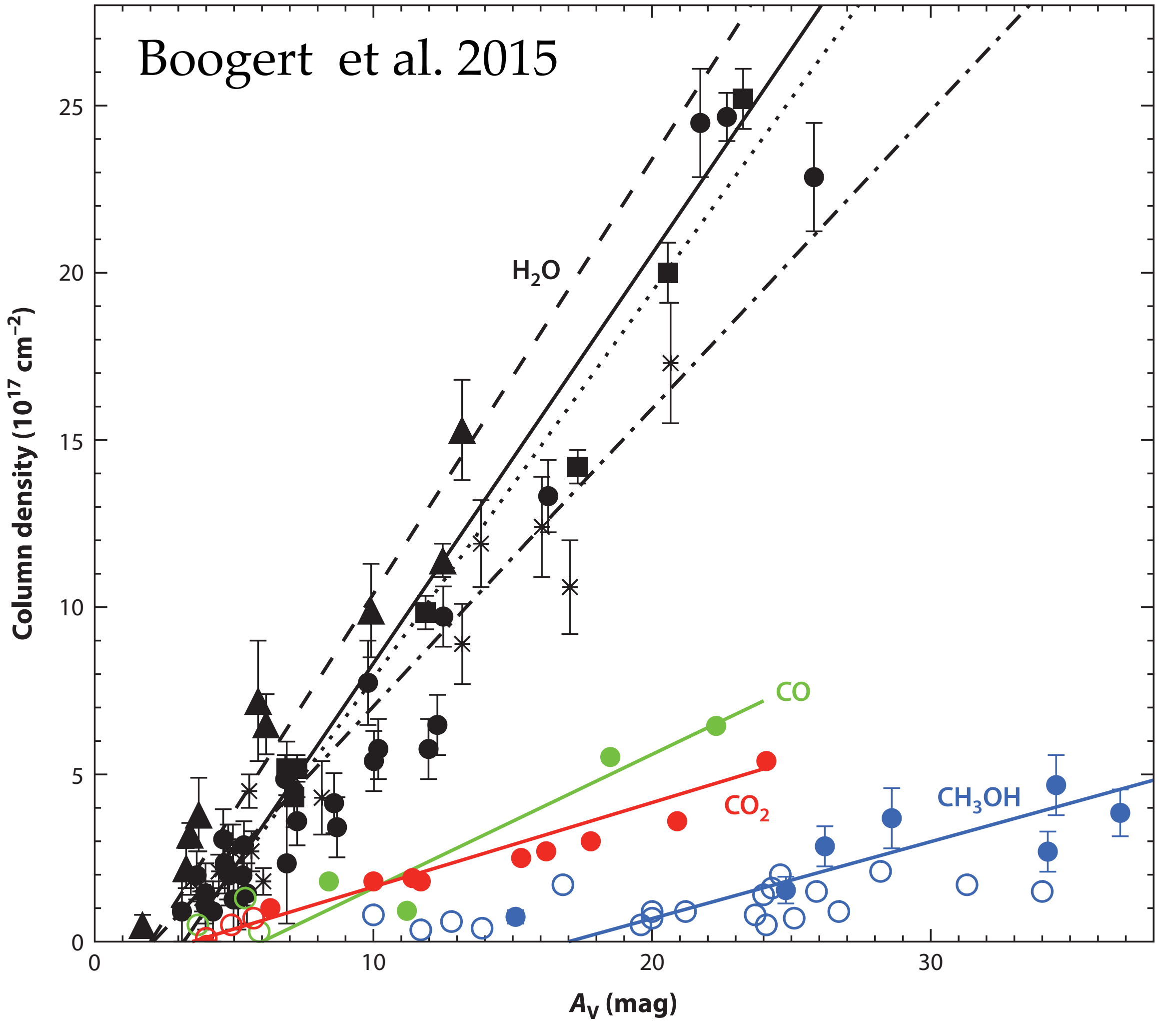


Boogert et al. 2015

Interstellar ices

Traced by their molecular vibrational transitions in the NIR and FIR: $\lambda \sim 1 - 100\ \mu m$

Mainly consist of H_2O, CO, CO_2, CH_4, NH_3, H_2CO and CH_3OH

Evidence for the presence of more complex molecules (e.g. HCOOH, CH_3CH_2OH, CH_3CHO, SO_2, N_2, O_2, HCN, OCS, …)

Diffuse / translucent clouds

Wide variety of simple molecules in the diffuse/translucent medium

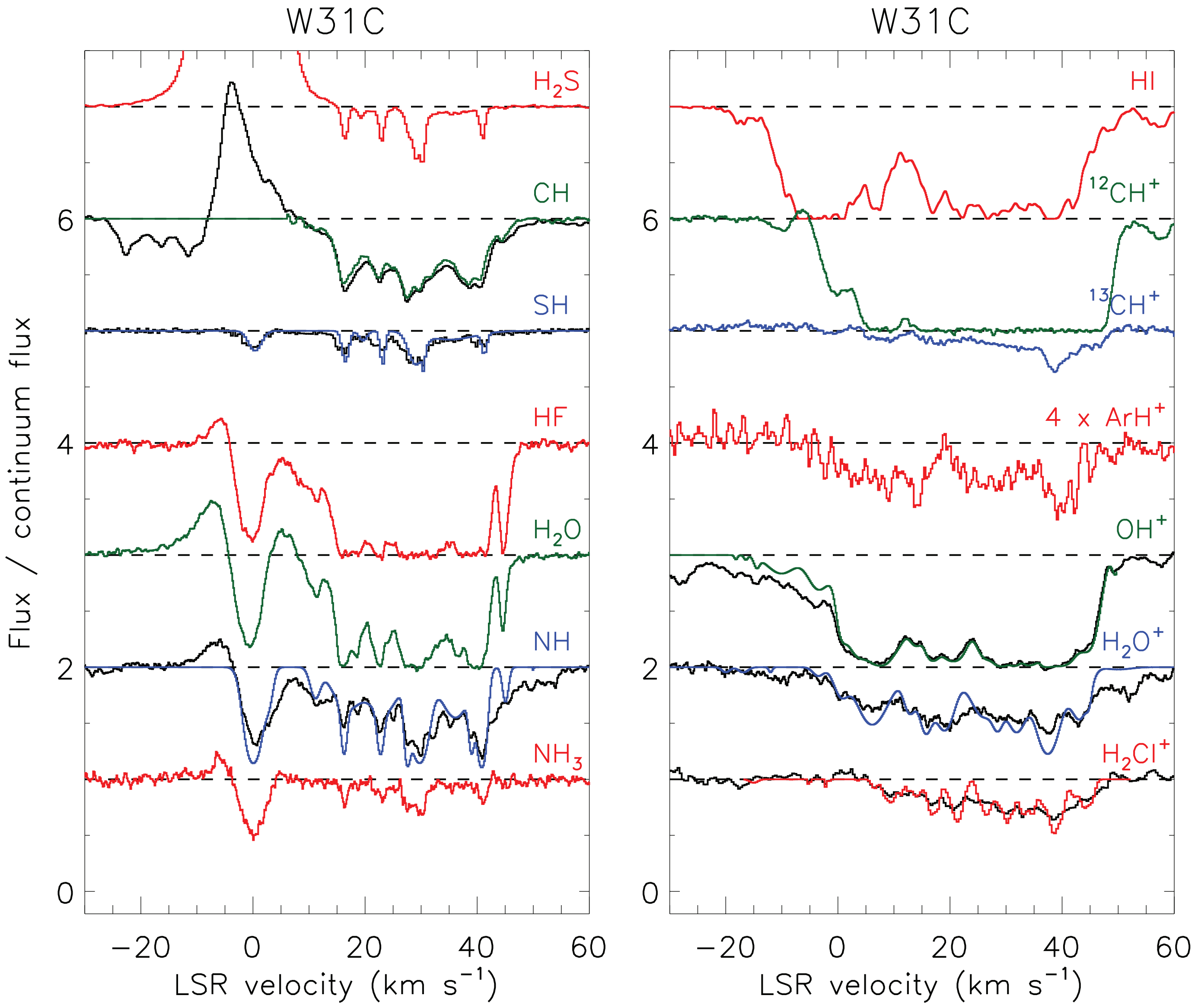
Herschel and SOFIA have provided a comprehensive view of FIR and sub-mm universe

- Velocity resolved observations
- New molecules: OH^+, H_2O^+, H_2Cl^+, ArH^+, …

More complex molecules are also present:

- Ubiquitous presence l-C_3H and CH_3CN (Liszt et al. 2018)
- Complex organic molecules (COMs) (Thiel et al 2017)

Gerin et al. 2016



Diffuse / translucent clouds

Most of these molecules have simple chemistry:

- Chemical model in relatively good agreement with most of the abundant molecules
- Robust tracers of the physical conditions

Balance between formation/destruction:

efficiency factor

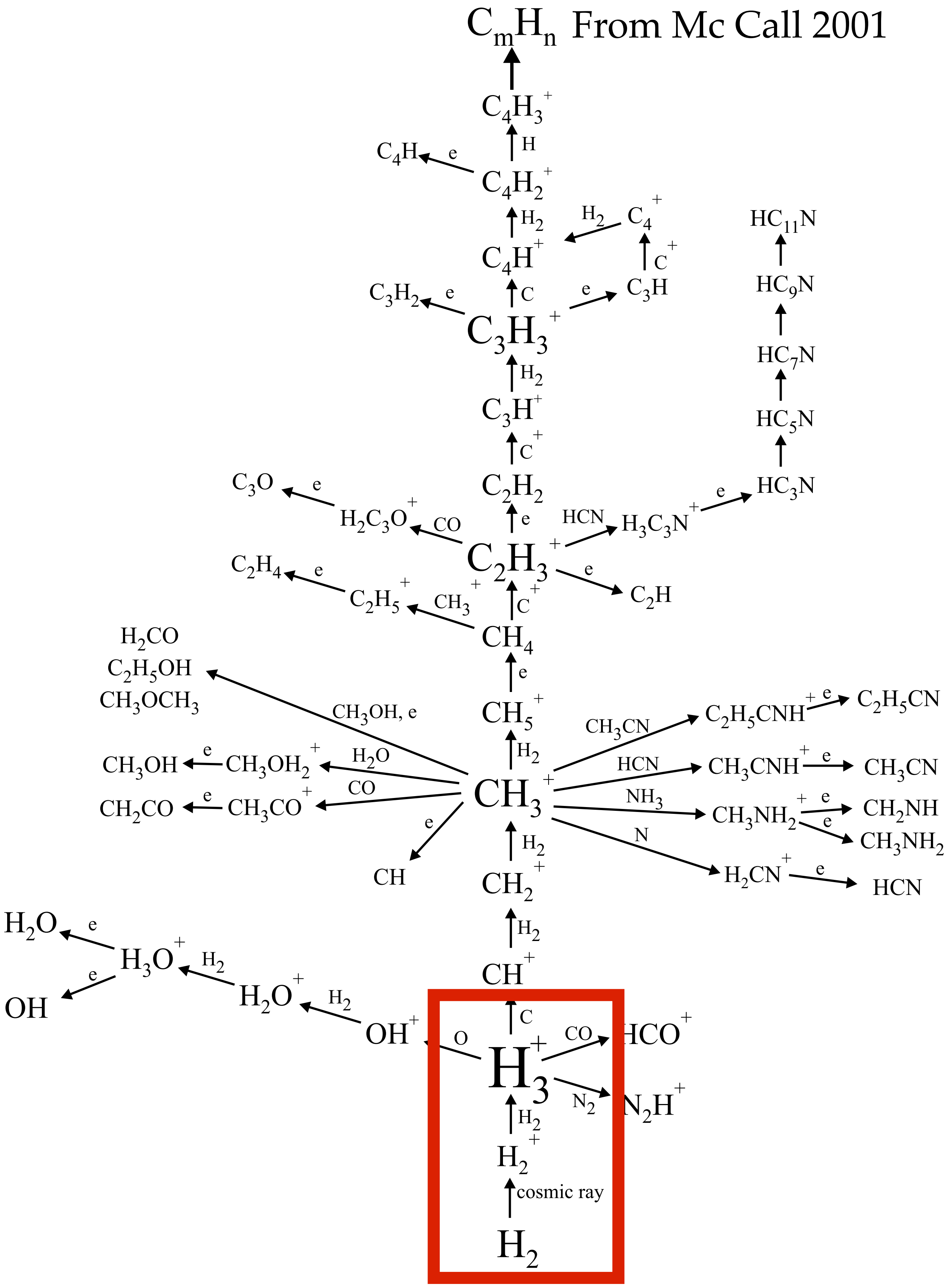
electronic fraction

$$\epsilon \zeta_{\mathrm{H}} = \frac{N(\mathrm{OH}^+)}{N(\mathrm{H})} n_{\mathrm{H}} x_e \left[\frac{k_7}{N(\mathrm{OH}^+)/N(\mathrm{H_2O}^+) - k_6/k_4} + k_5 \right],$$

Cosmic ray ionisation rate

$\zeta_H \sim 10^{-16}\ s^{-1}$ in diffuse clouds

➔ confirm estimation based on H_3^+

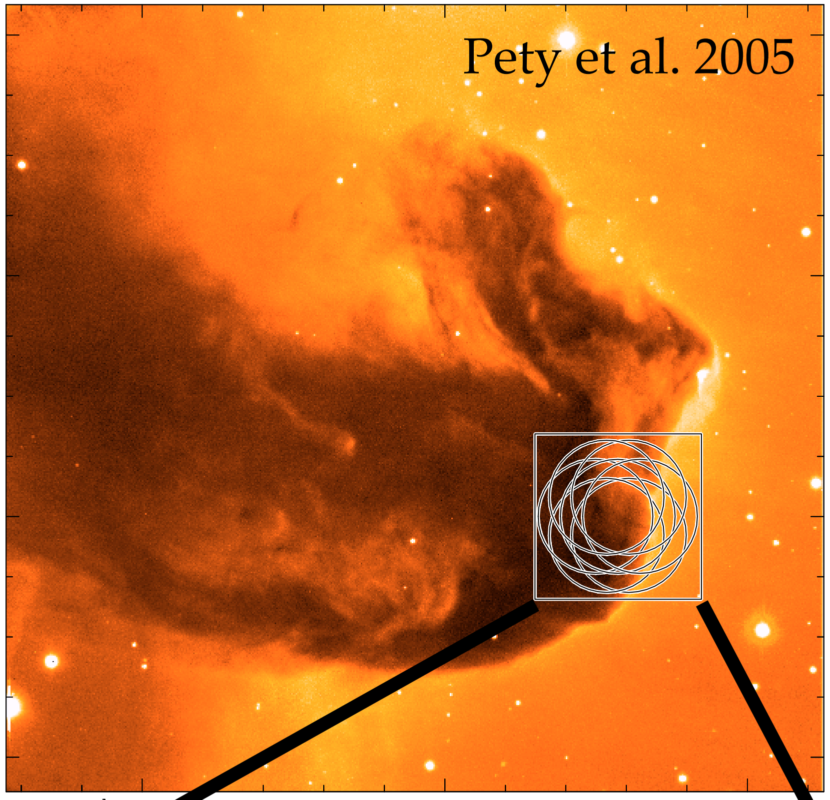


From Mc Call 2001

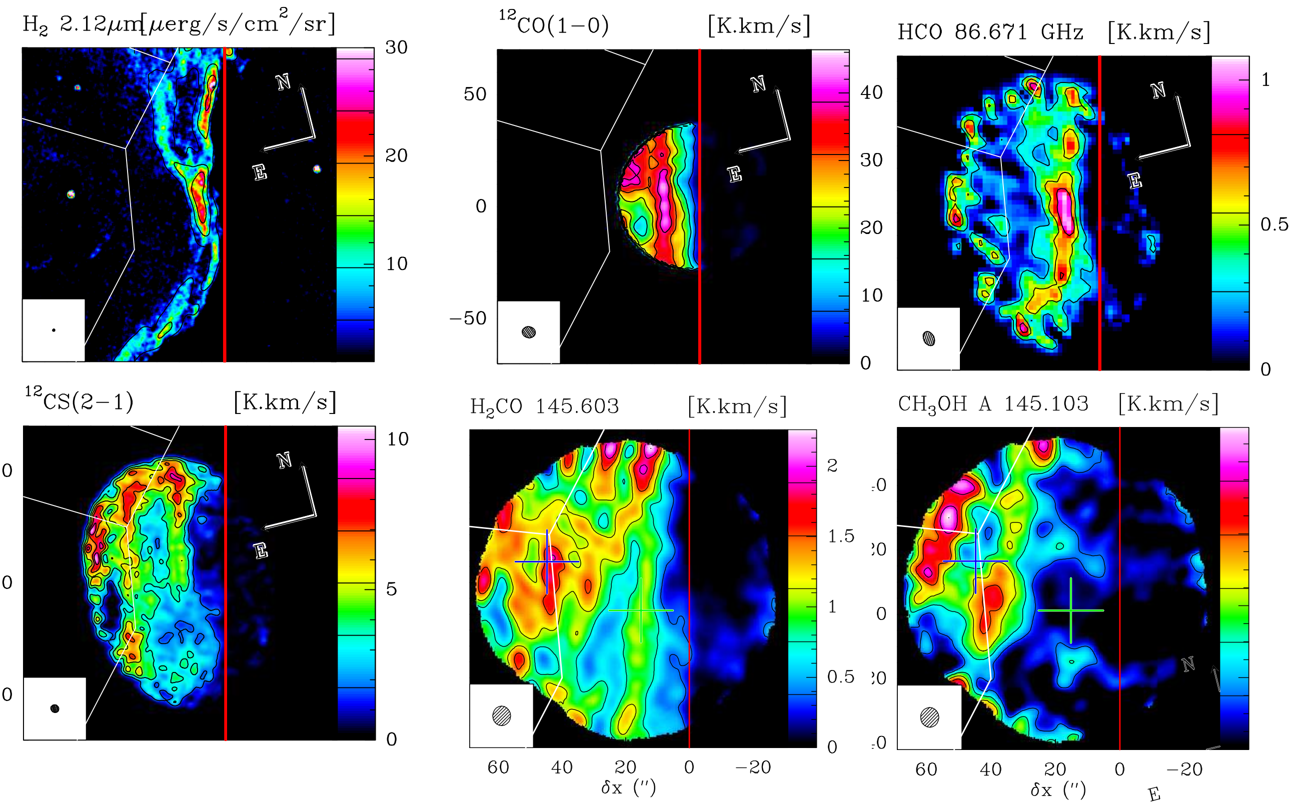
Physics and chemistry in PDRs

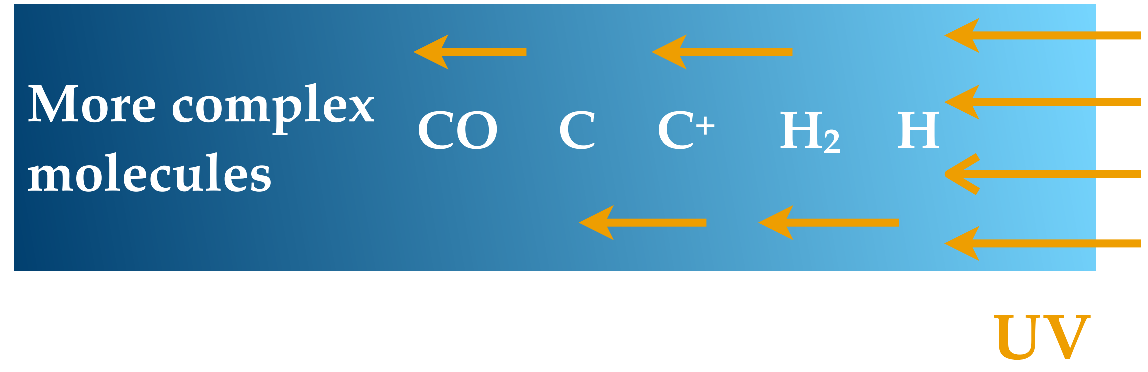
PDRs are good target to test our understanding of the physics and the chemistry:

- Many of the physical and chemical processes that regulate diffuse clouds are identical to those in dense PDRs
- High surface brightness
- Spatially resolved



Pety et al. 2005





More complex molecules CO C C^+ H_2 H

UV

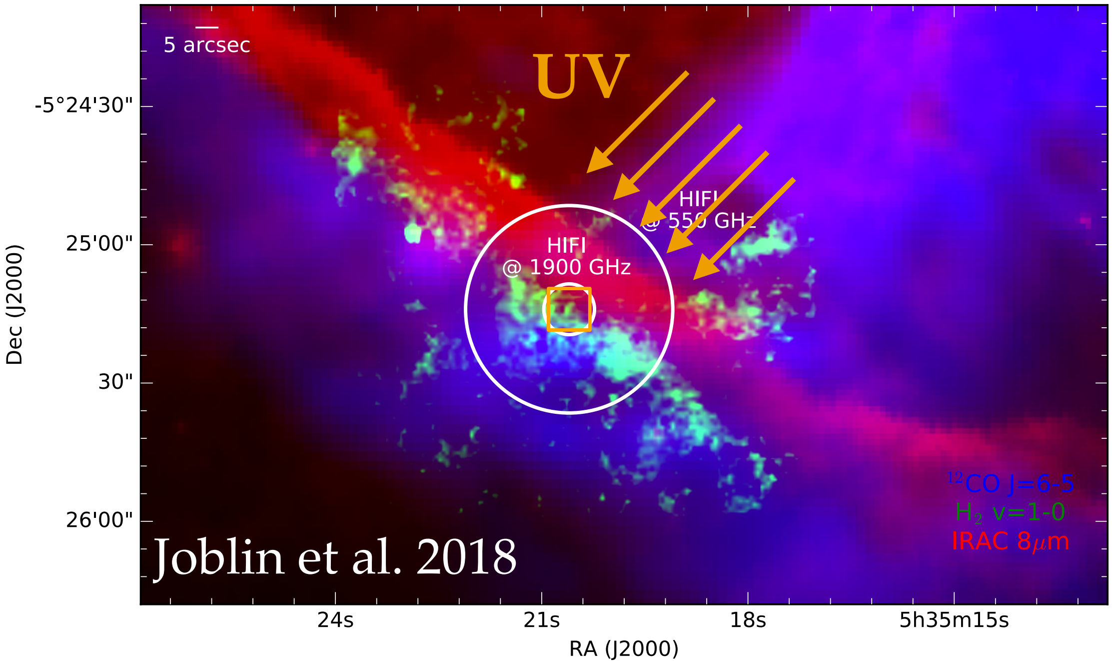
Physics and chemistry in PDRs

Models of PDRs:

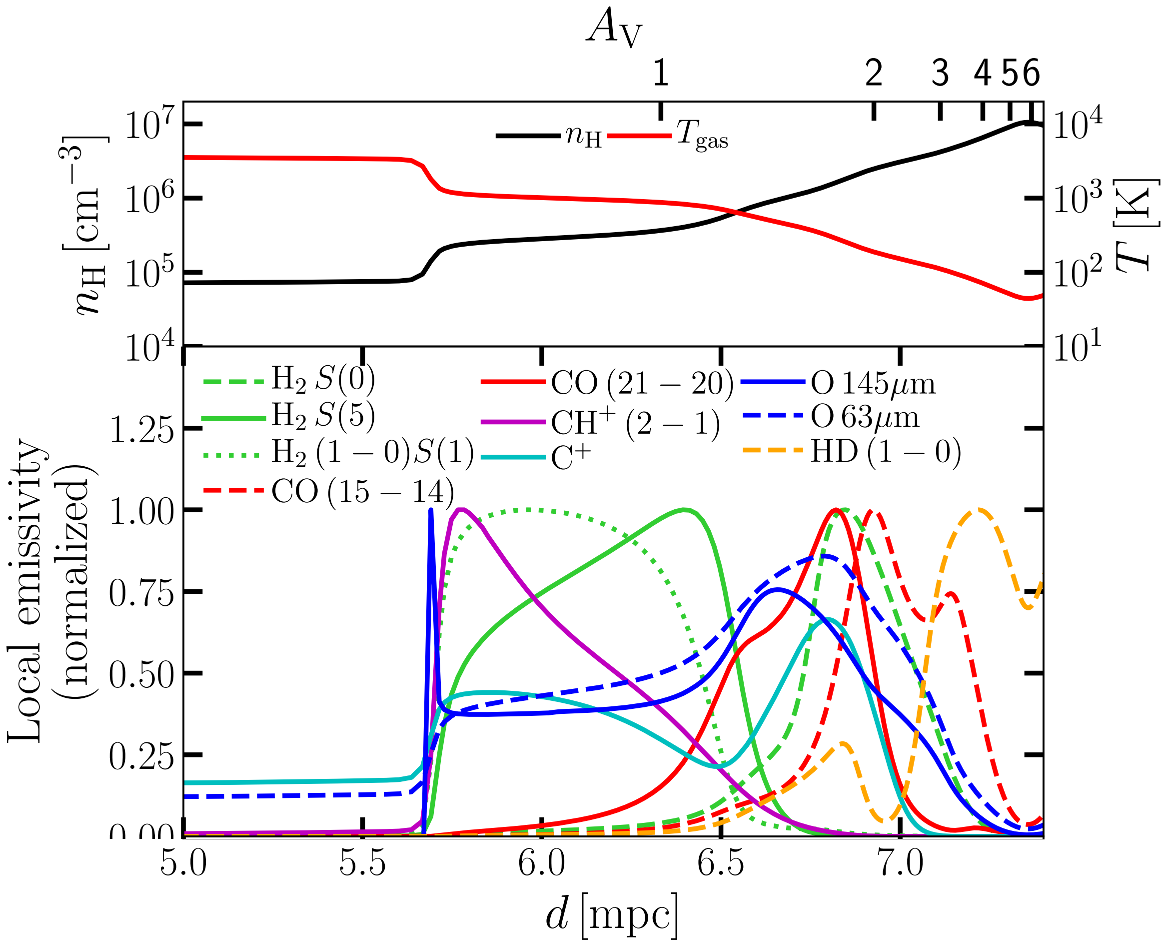
- Micro-physics treated in great details
- Thermal balance, chemistry and radiative transfer equation are coupled and solved iteratively

We get:

- Physical structure
- Molecular abundance
- Line and continuum intensities that can be directly compared to observations



Joblin et al. 2018



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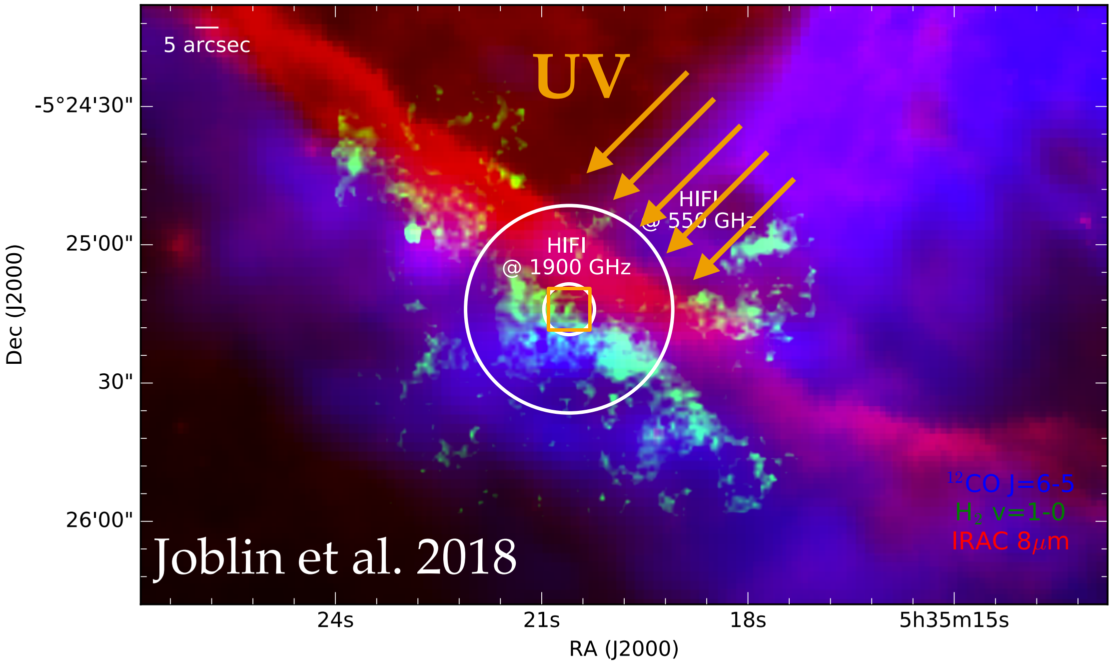


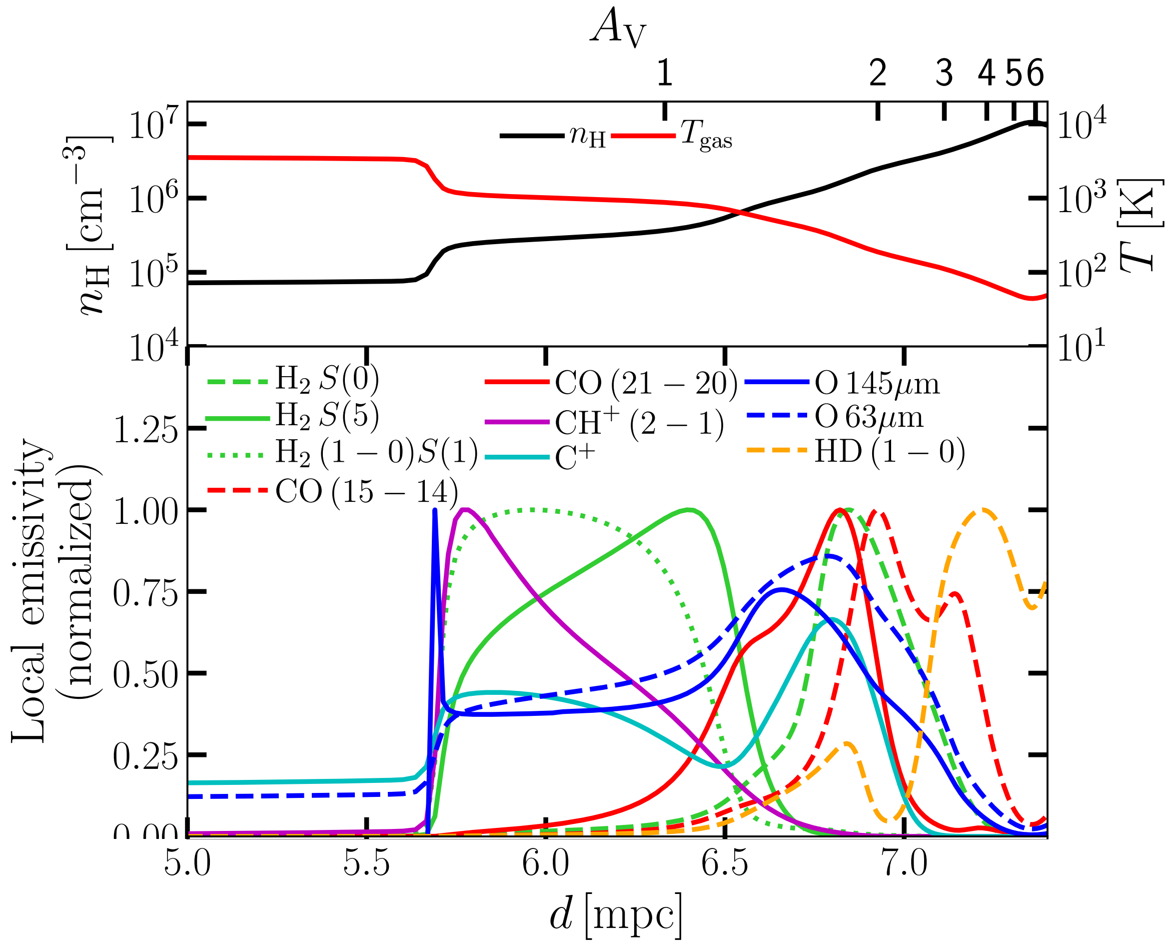
Joblin et al. 2018

We get:

- Physical structure
- Molecular abundance
- Line and continuum intensities that can be directly compared to observations

Difficult to have a complete view on the evolution based only on these models:

- Dynamical effects are generally neglected
- Chemistry assumed to be at equilibrium in most of the case. Good approximation when $t_{chem} < t_{dyn}$ ➔ Do not hold in dense and shielded regions where $t_{chem} \sim t_{dyn}$.

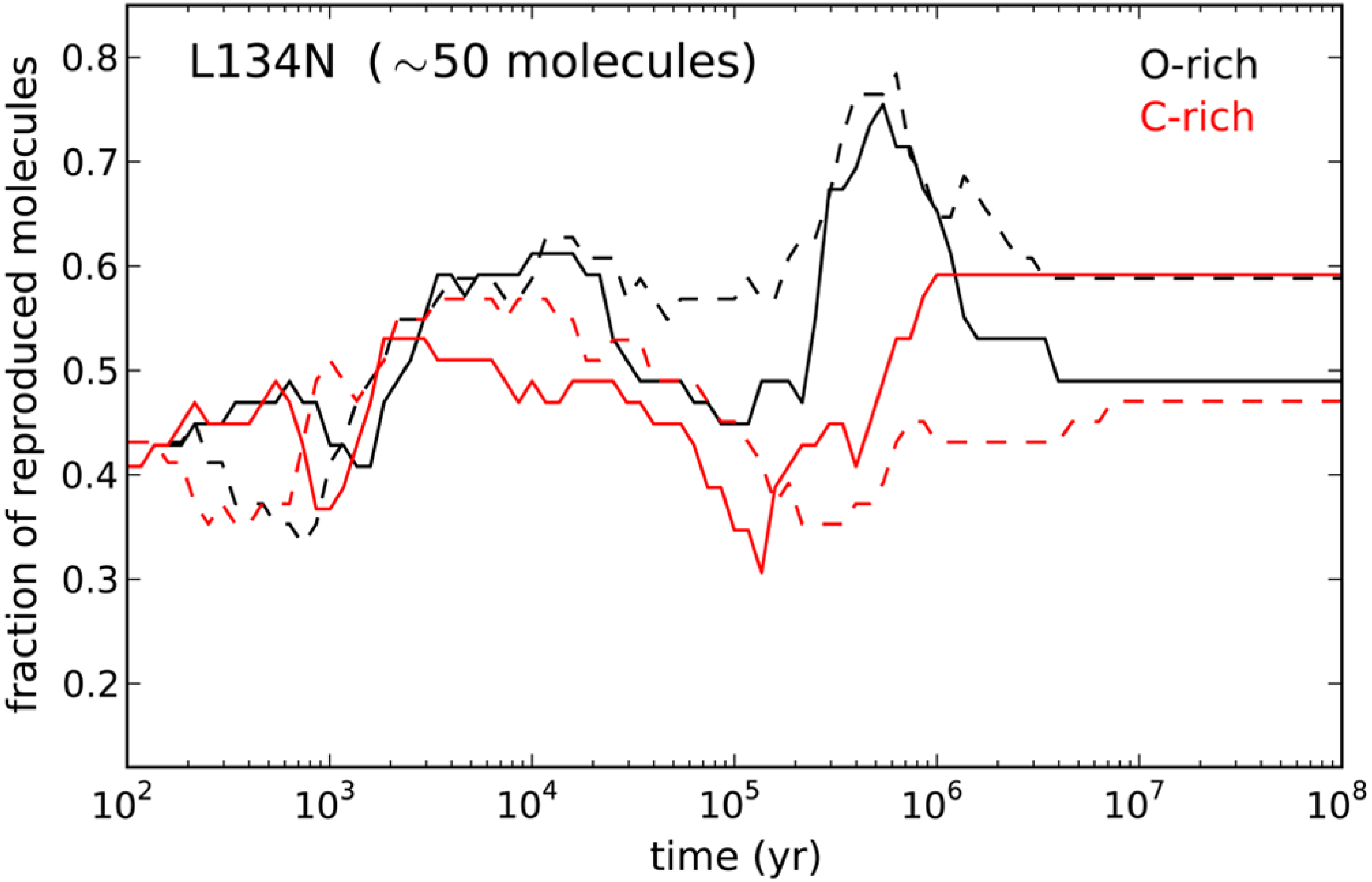


Chemistry of cold dark clouds

Pseudo-time dependent chemical models

- Solve the chemistry as a function of time
- Chemistry in cold dark clouds is pretty well understood

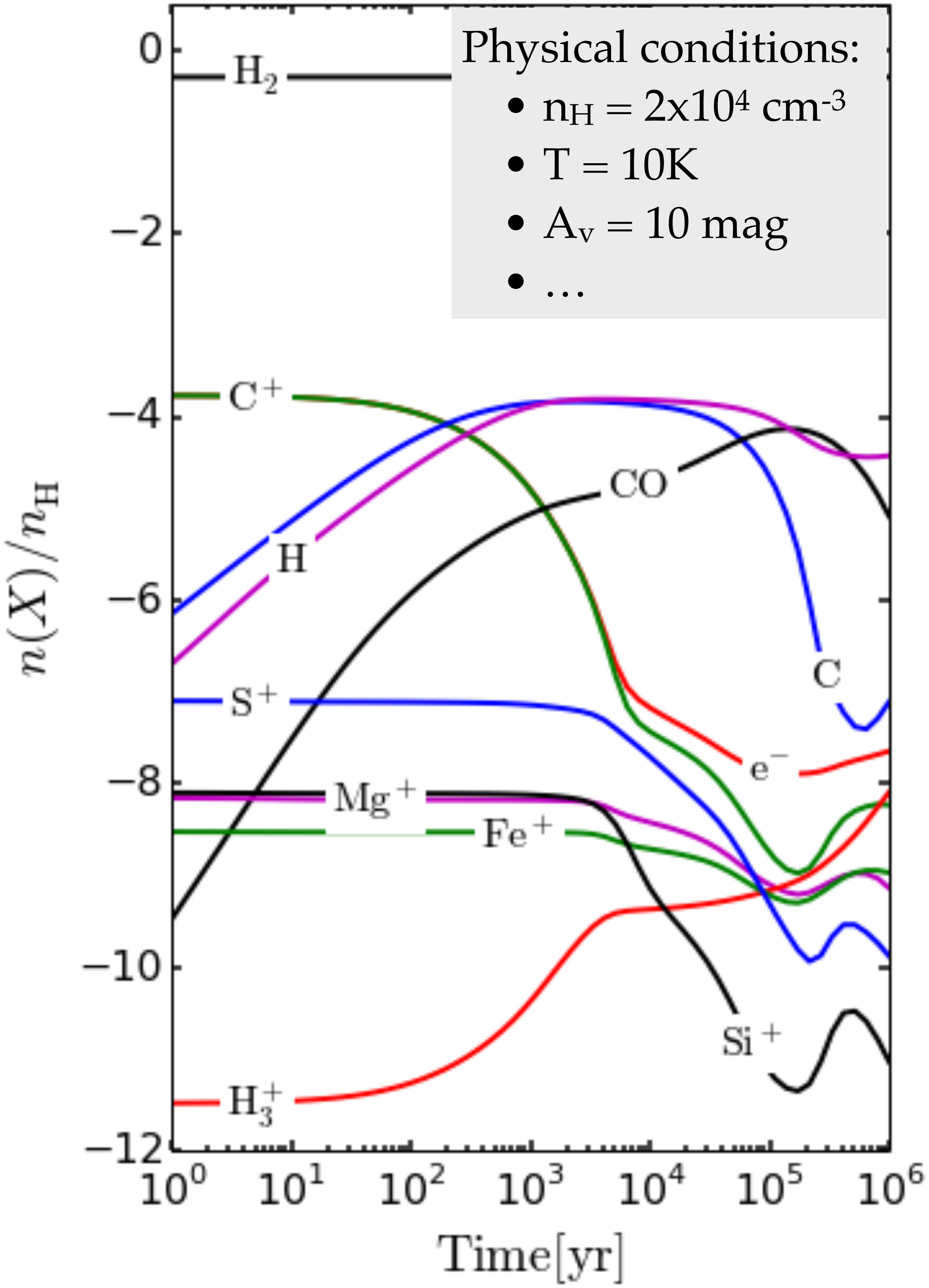
Agúndez & Wakelam 2013



Chemistry of cold dark clouds

But strong assumptions on the transition between diffuse and dense medium…

- Dark clouds often considered as simple objects: physical conditions assumed to be constant
- "low-metal abundances" (Graedel et al. 1982)
- No inherited molecules from the diffuse medium ➔ Could have lead to the controversial idea of an early time chemistry in some of dense clouds (e.g. TMC-1)


Physical conditions:

- $n_H = 2x10^4$ cm^{-3}
- T = 10K
- $A_v = 10$ mag
- …

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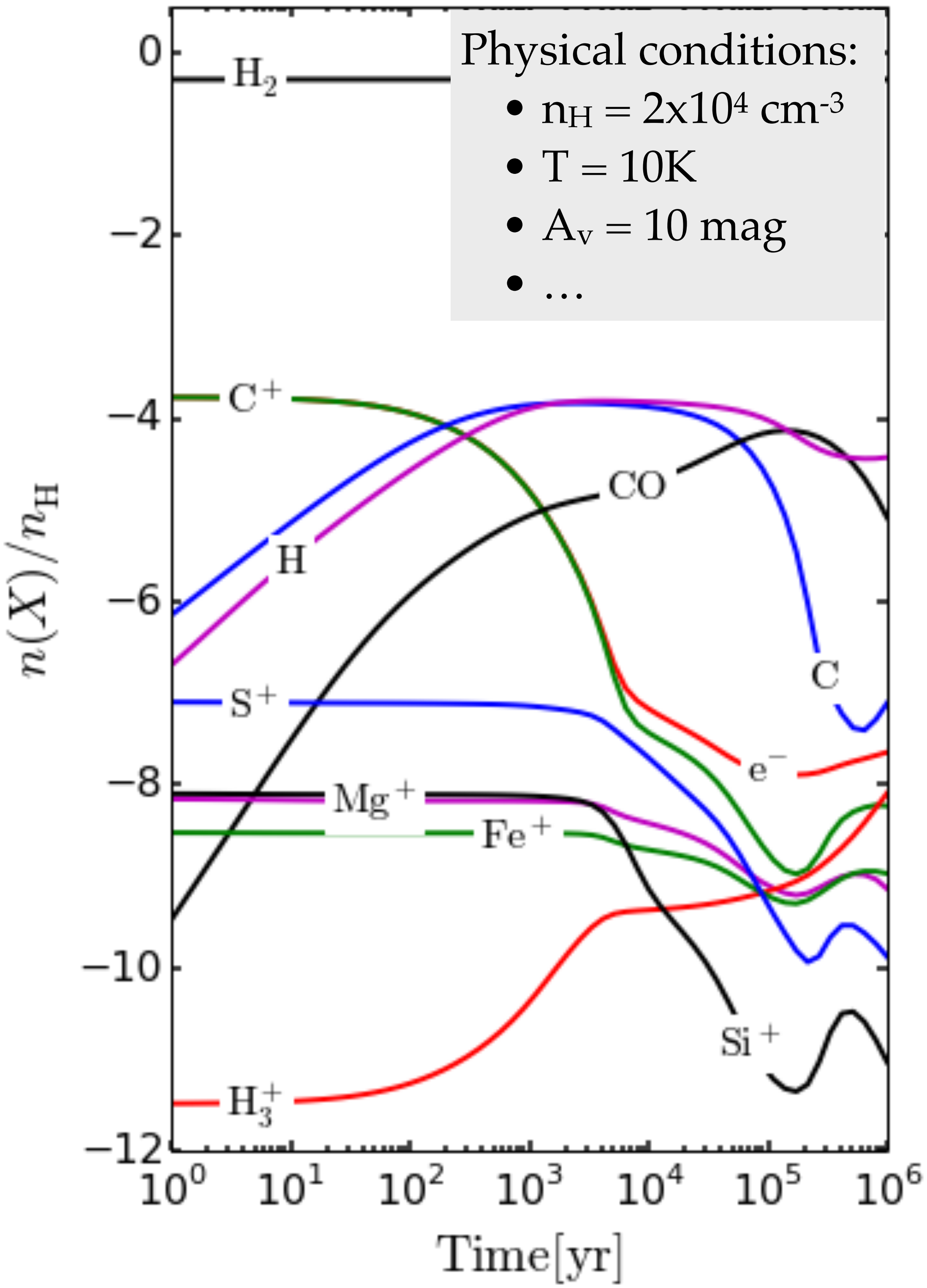
Reflect the lack of information on their dynamical history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From diffuse to dense clouds

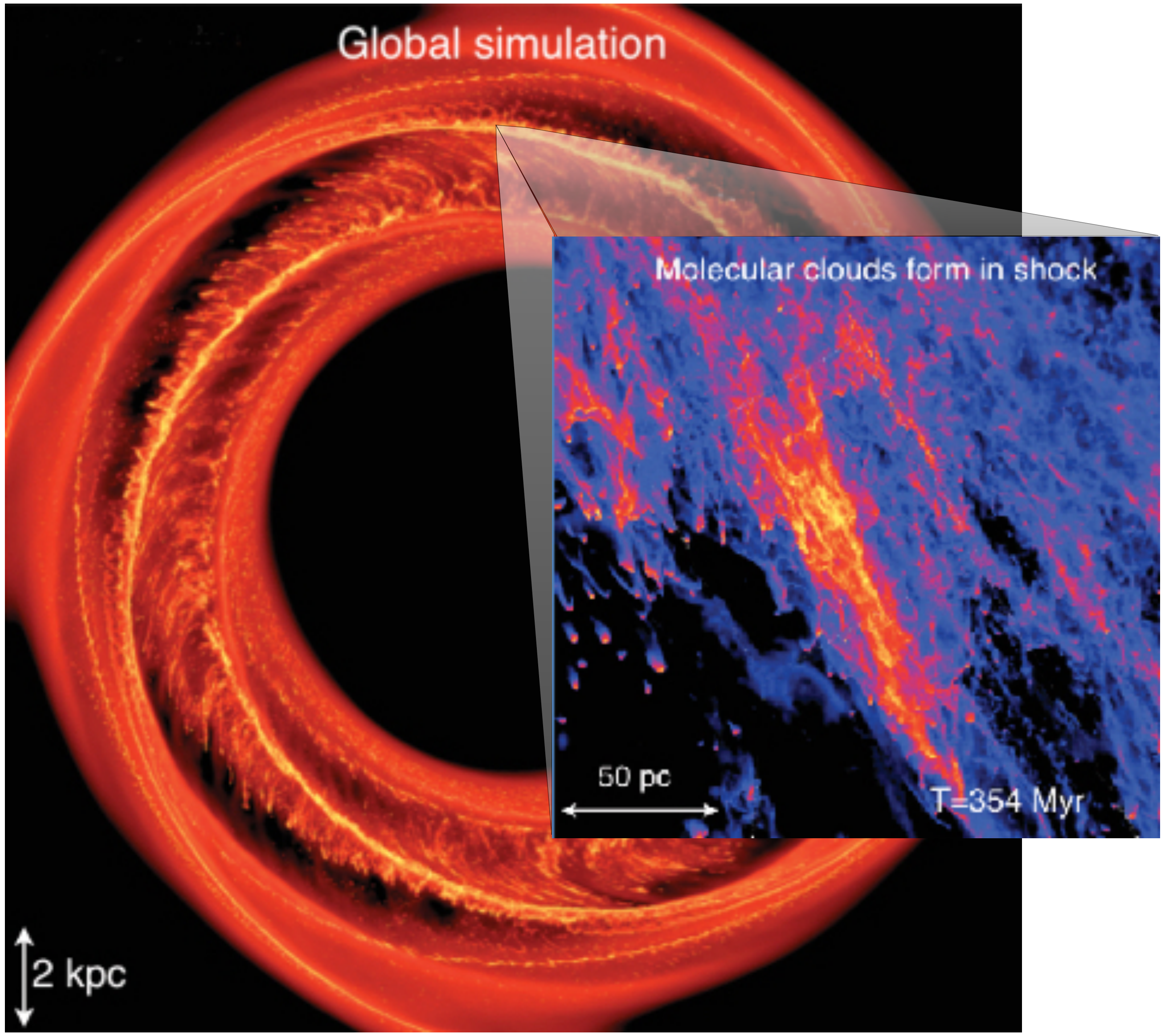
Follow the evolution of the chemical composition of dense clouds from the diffuse ISM (Ruaud et al. 2018)

- Chemistry as a post treatment of the dynamics
- No assumptions on the initial abundances: typical from the diffuse ISM
- Possibility to use a complex time-dependent chemical model (gas + grains)

From diffuse to dense clouds

Large scale hydrodynamic simulation

- 3D SPH simulations
- Top down approach used to probe successive smaller scales
- Dense clouds formed by converging flows induced by shocks when the matter enters the spiral arm potential
- High resolution re-simulation: evolution of a parcel of gas 250x250pc^2
    - 10^7 particles de 0.15M⊙ each
    - Period de 50 Myr (~1/4 of a galactic orbit)

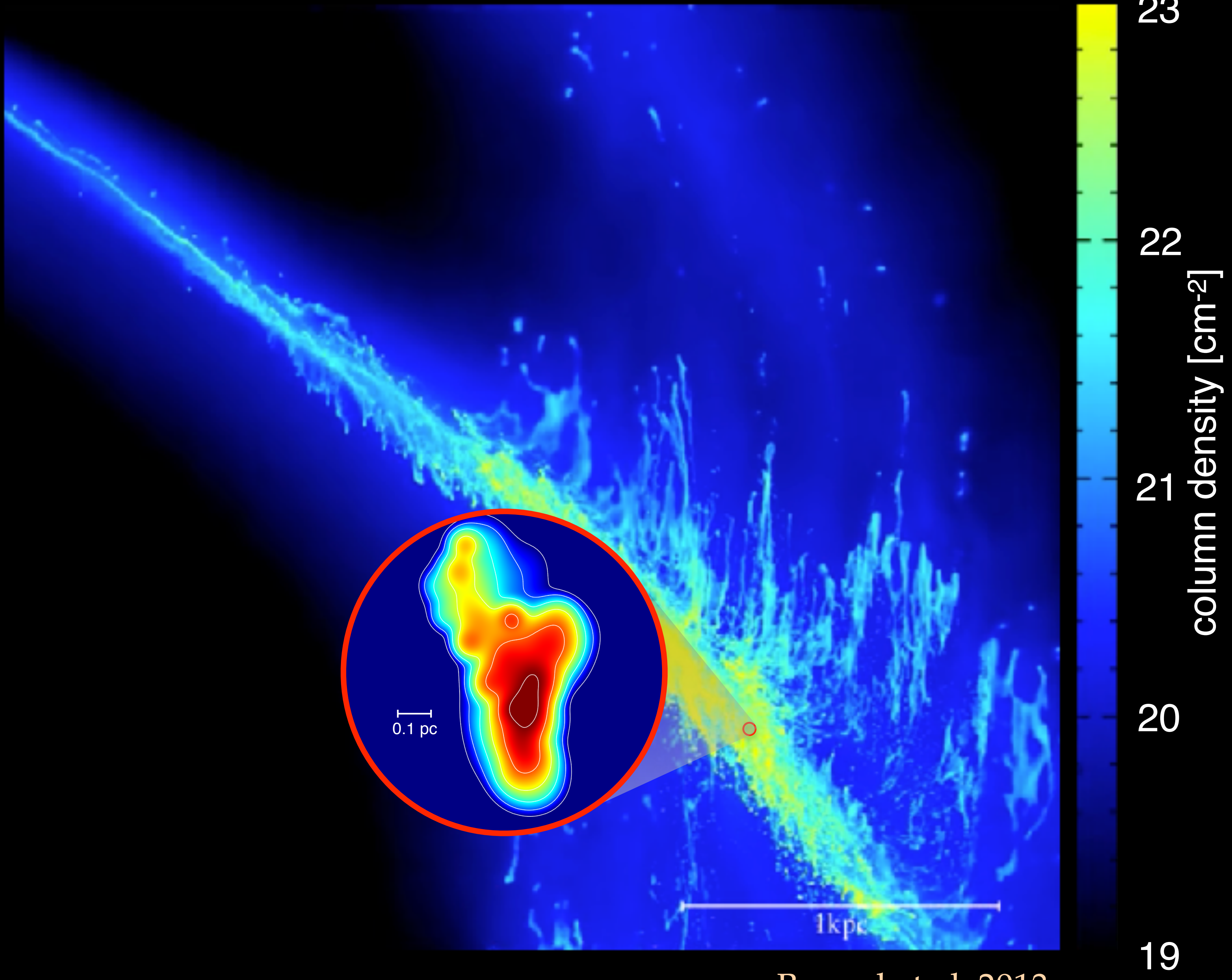


SPH simulations from Ian Bonnell
(Bonnell et al. 2013)

From diffuse to dense clouds

Method

- Selection of some dense clouds and extraction of the physical history of each SPH particle that form them



Bonnel et al. 2013

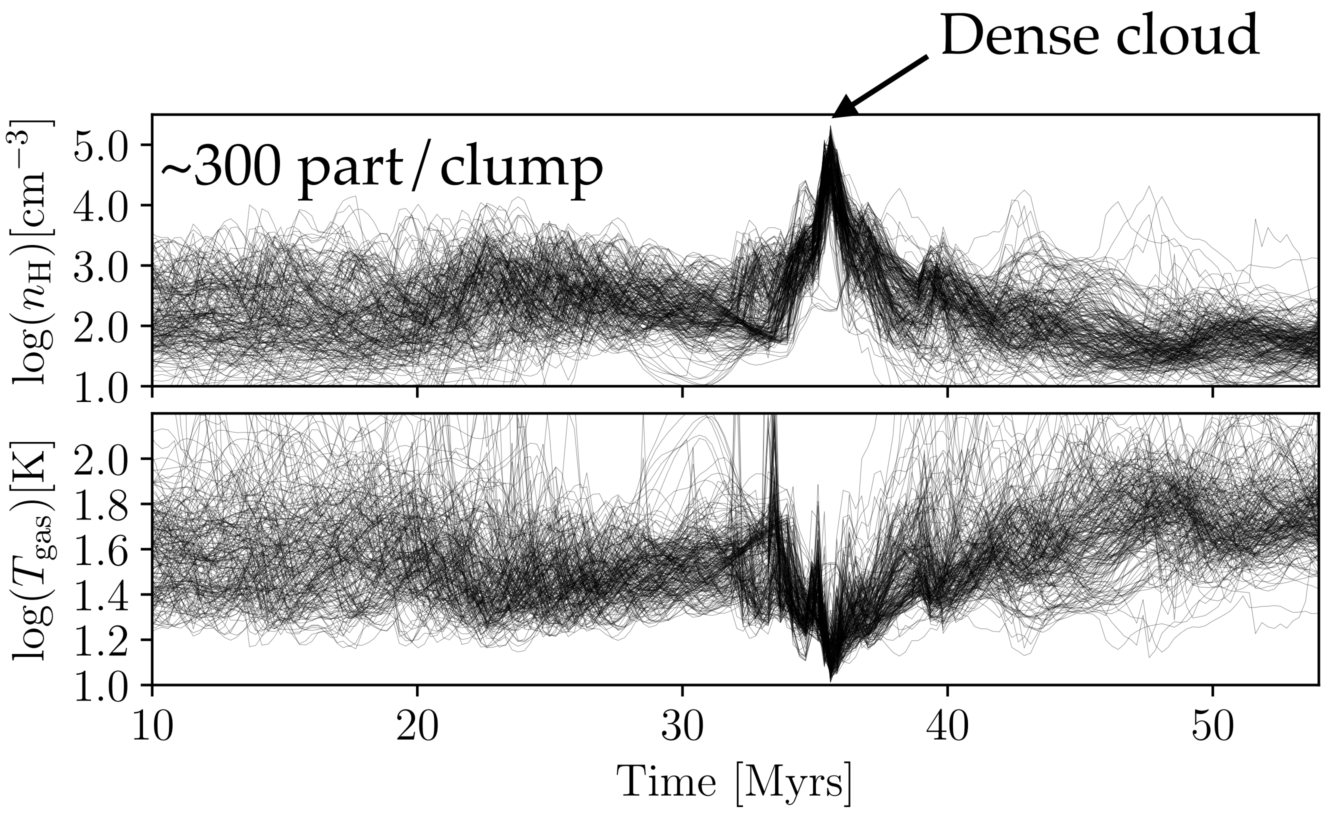
From diffuse to dense clouds

Method

Extraction of $n_H(t)$, $T_{gas}(t)$ and Av(t) for each SPH particles

Input of a full gas-grain chemical model (Nautilus, Ruaud et al. 2016):

- ~700 chemical species (500 for the gas and 200 for the grains)
- ~10000 reactions



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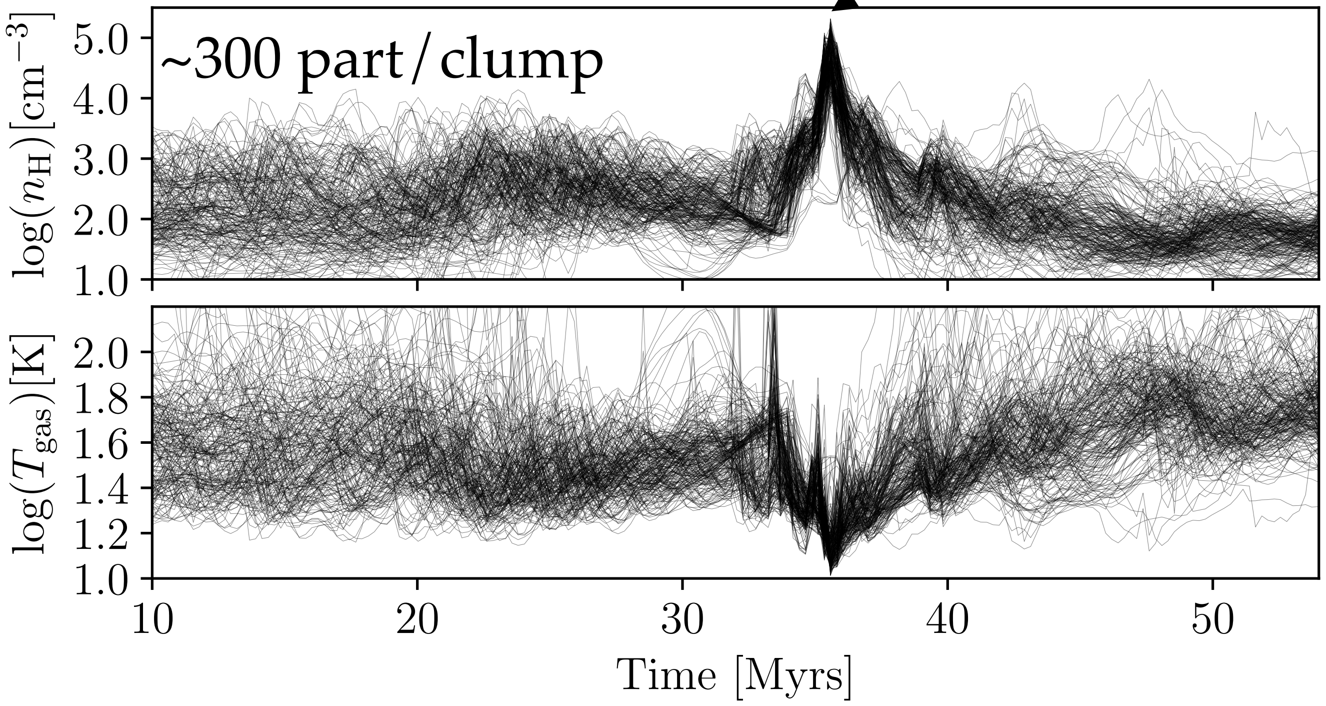
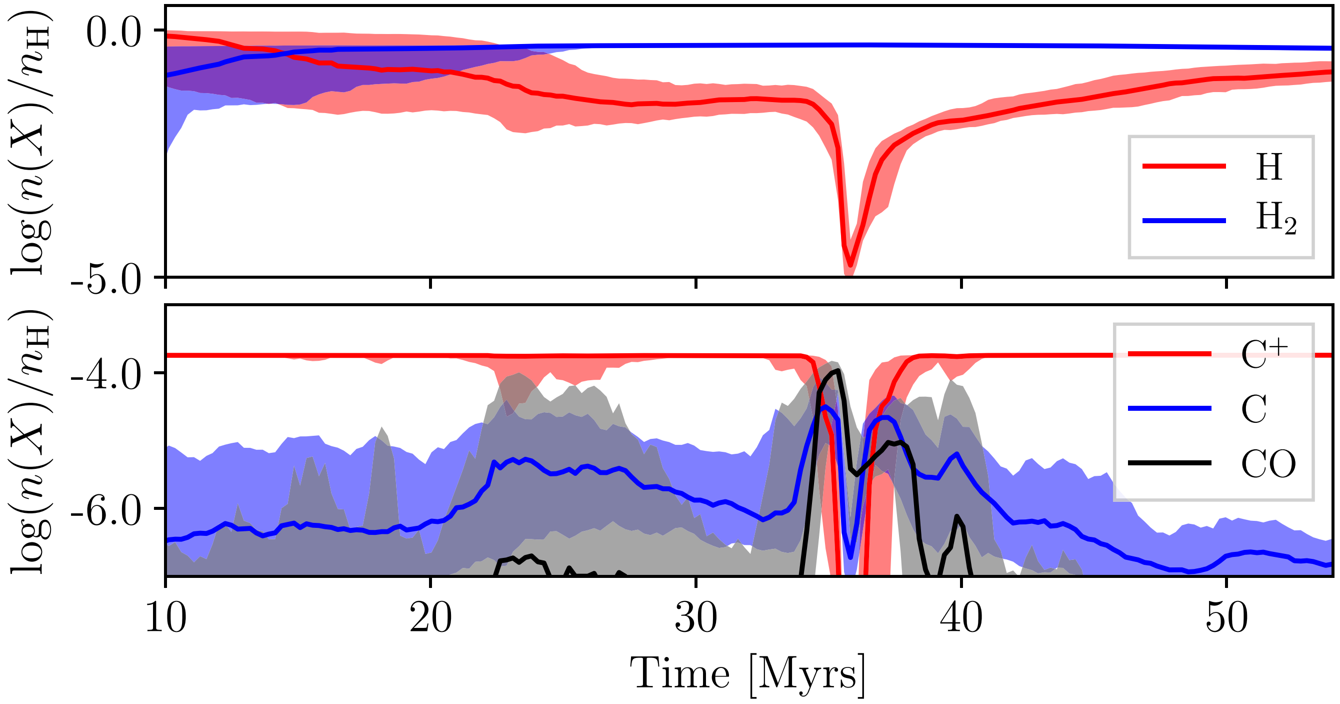
We follow the evolution of the chemical composition from the diffuse ISM up to the formation of the dense cloud

Dense cloud





Ruaud et al. 2018

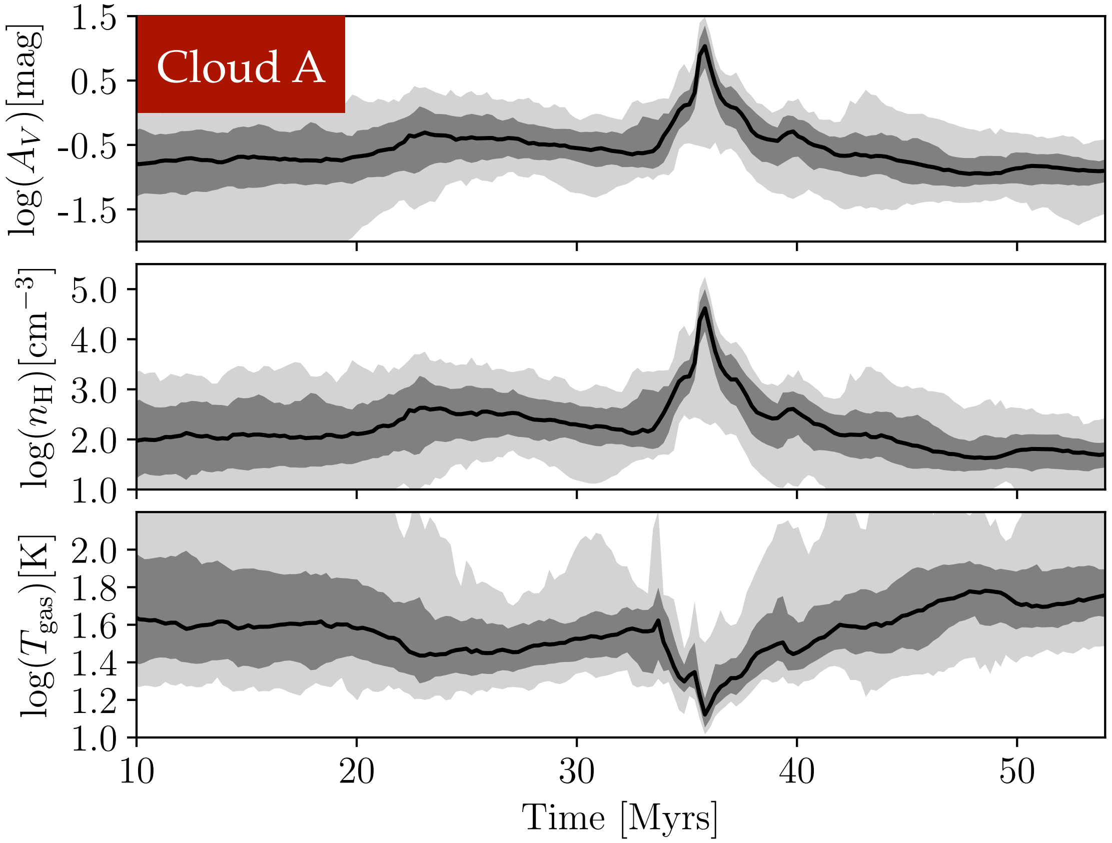
From diffuse to dense clouds

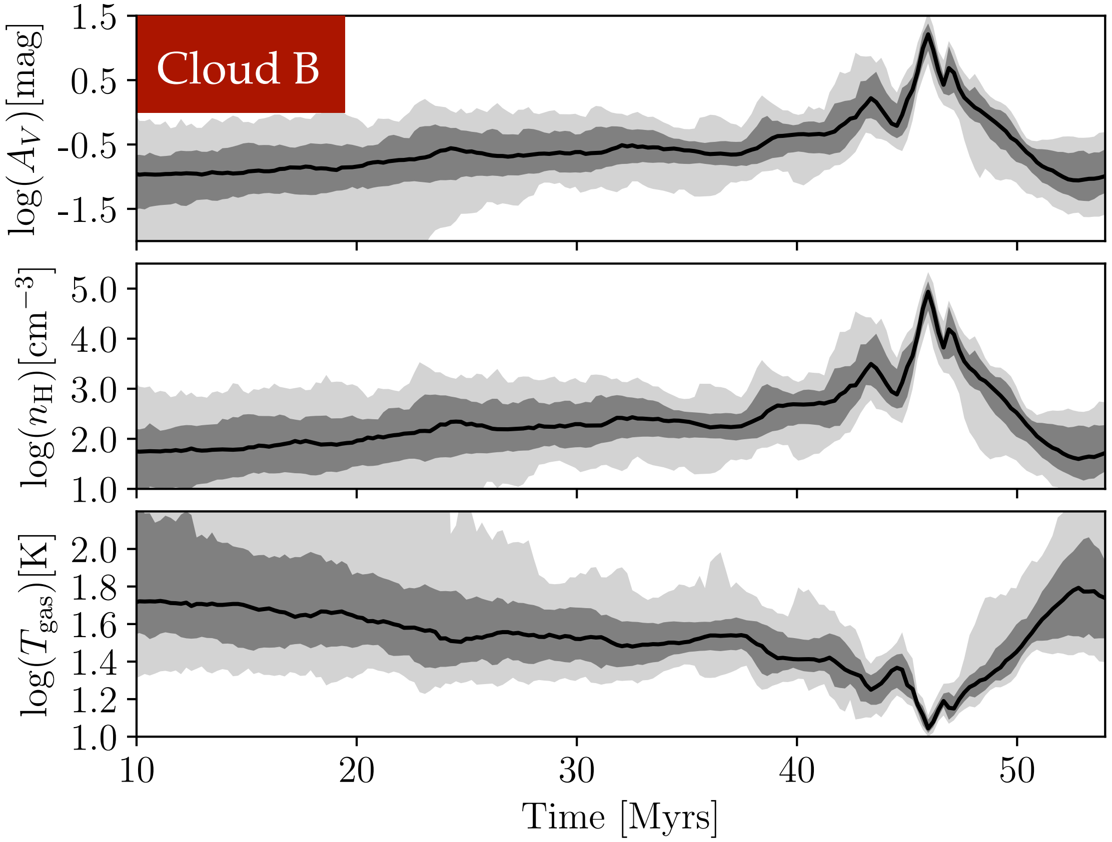
Results for two clouds

Selection motivated by:

- Similarity of the physical parameters in the dense cloud regime
- Different physical history

	Cloud A	Cloud B
Number of SPH particles	237	287
Total mass ($M_\odot$)^a	37	45
Mean radius (pc)	0.33	0.29
Velocity dispersion (km s^{-1})	1.4	0.7
Virial parameter^b	20.0	4.0
Median T_{gas} (K)	12.0	11.0
Median n_H (cm^{-3})	4×10^4	7×10^4



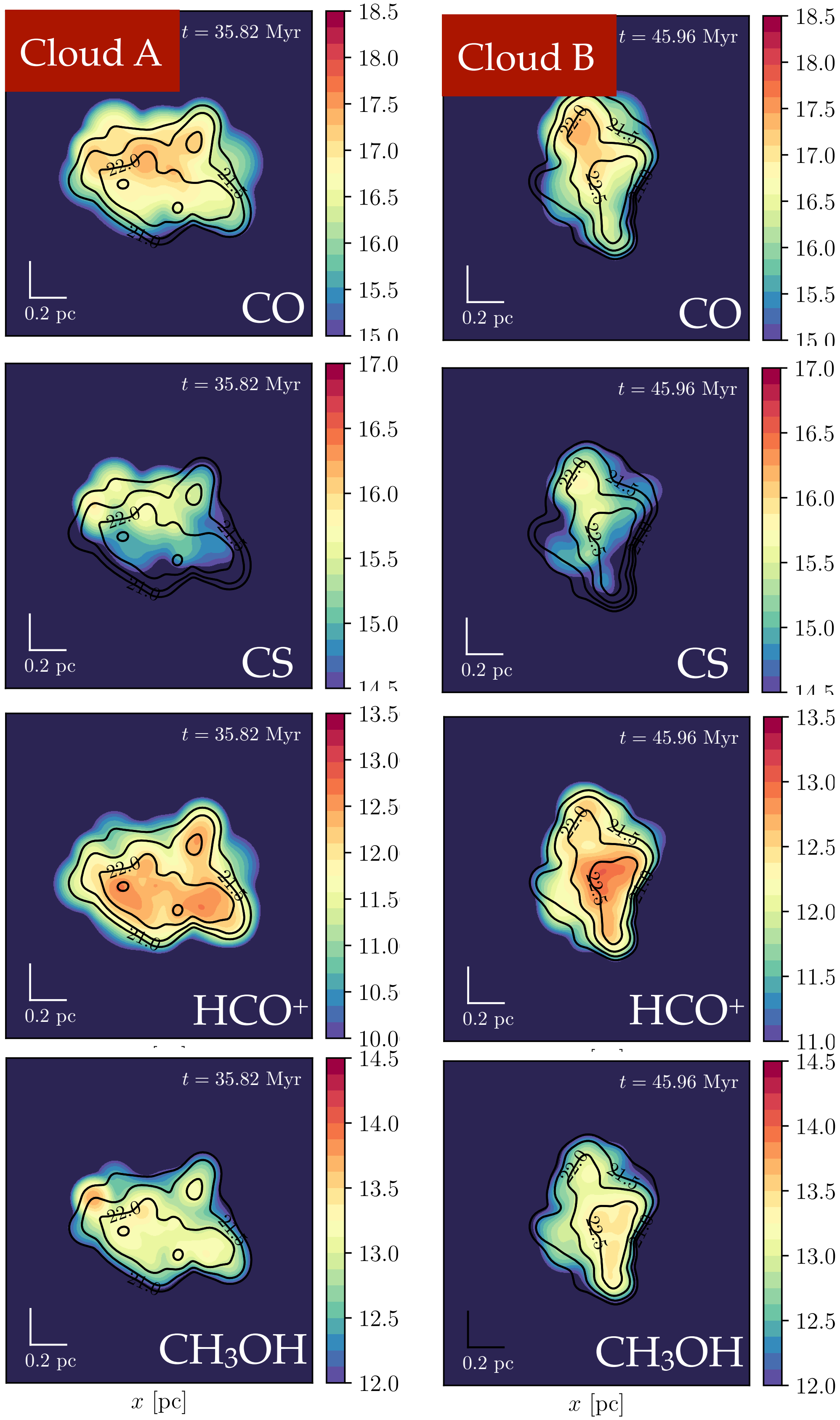


From diffuse to dense clouds

Results for two clouds

Similar results for most of the commonly observed molecules:

- Depletion of some molecules in the densest part of each clouds (e.g.: CO and CS)
  - ➔ Abundance gradient on small spatial scales
- Molecule like CH_3OH does not show any sign of depletion and is well distributed
  - ➔ Formation on grains allow the continuous replenishment of the gas-phase



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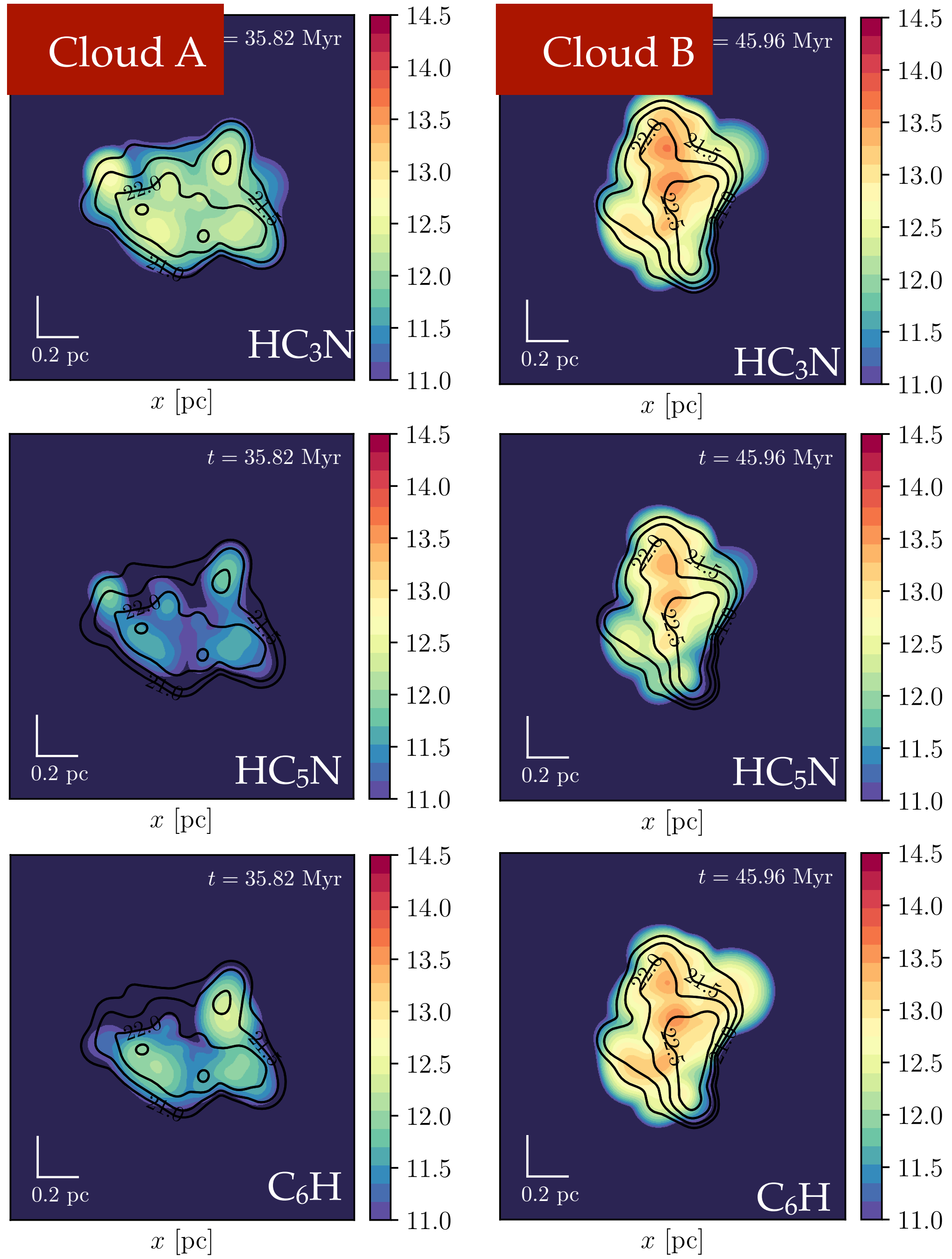


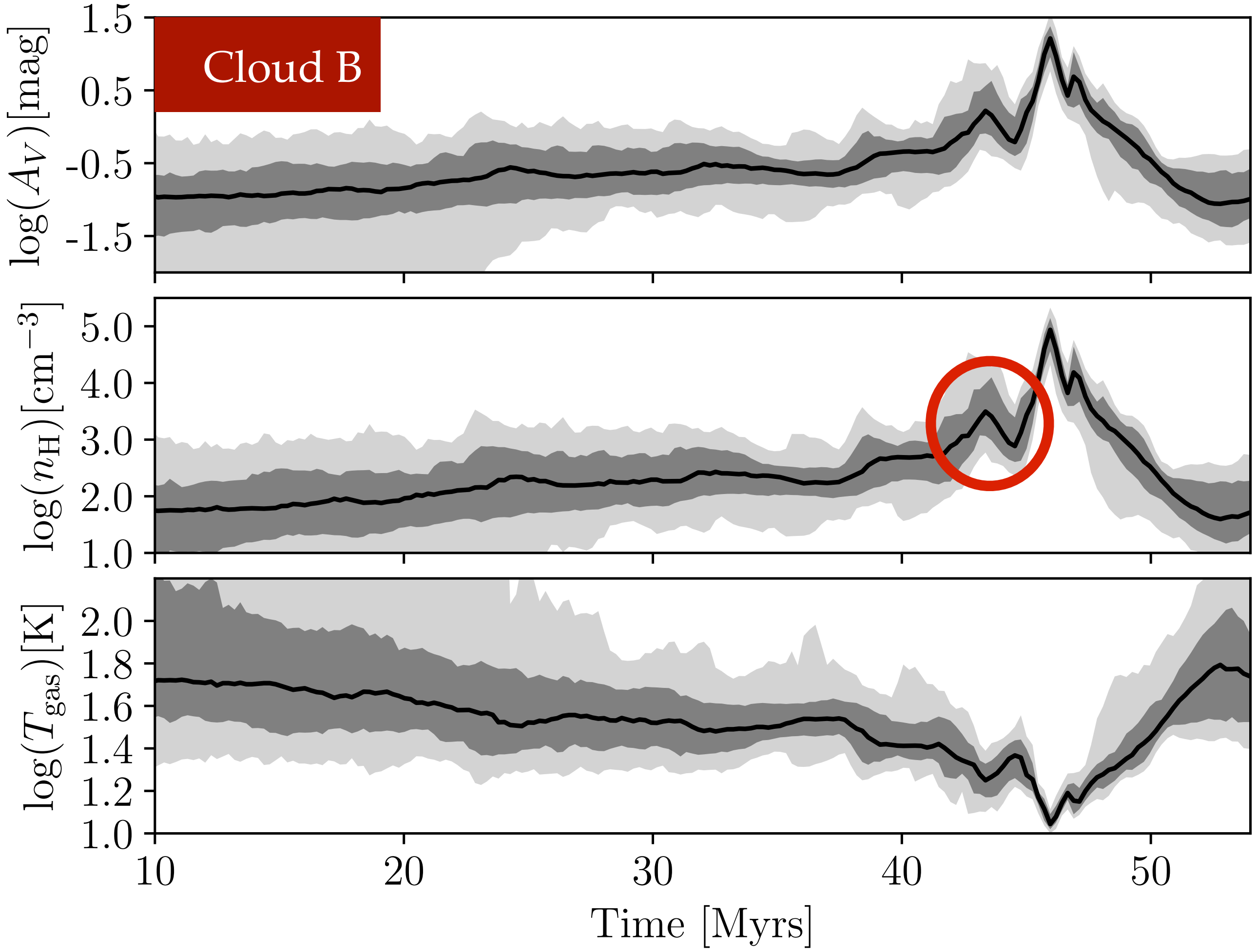
Strong differences for some molecules: mostly carbon chains

From diffuse to dense clouds

Results for two clouds

Presence of a density pre-phase in the case of cloud B:

- Depletion of the electron donors: reduces the electronic fraction ➔ Promotes the ion-chemistry
- Formation of H_2O on grains increases the gas-phase C/O ratio: more carbon is available



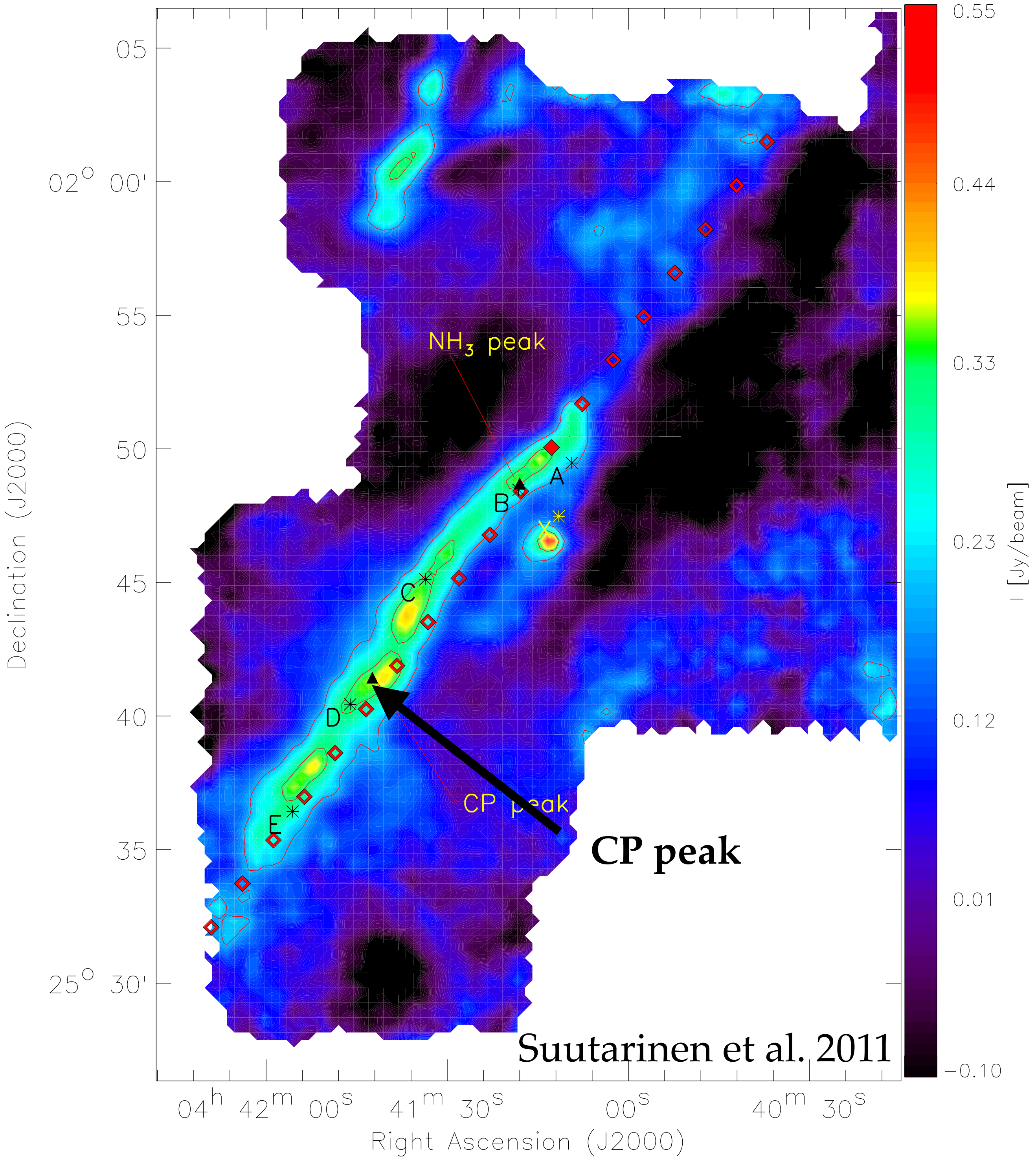
Carbon chains are efficiently formed

From diffuse to dense clouds

Enhancement of carbon chains in the TMC-1 (CP) dark cloud

Carbon chains and cyanopolynes are ~10x more abundant as compared to other similar clouds

- Uncertain origin: Most popular scenario based on the idea of an "early-time chemistry"
- Could be the results of the dynamics: some of the gas could have experienced a past density phase



CP peak

Suutarinen et al. 2011

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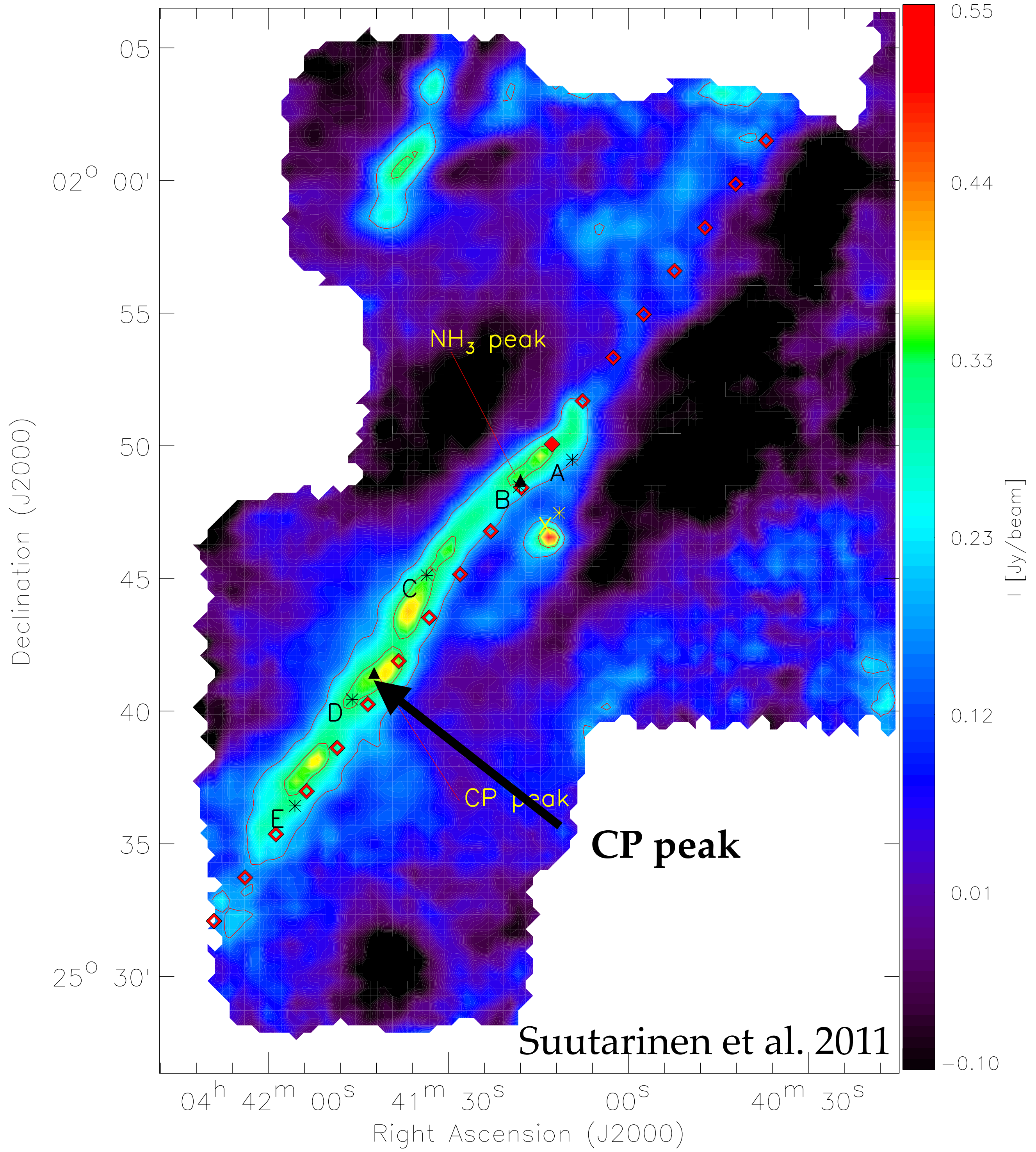
Changes significantly the story…



CP peak

Suutarinen et al. 2011

To summarize

- The ISM is a rich environment where physics and chemistry are strongly coupled
- MHD simulations show that the ISM is constantly evolving and strongly linked to its environment
- PDRs give insight on the physical and chemical evolution from diffuse to molecular clouds. But:
  - Dynamics not included in models
  - Chemical equilibrium is often assumed
- Dynamics is important and can impact the molecular composition
- Difficult to couple dynamics and chemistry properly: Computationally expensive to include in MHD simulations
- Post-processing of the chemistry on MHD simulations can help

Thank you for you attention