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Chemistry and dynamics in RAMSES:
post-processing tool towards a real coupling

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Why we should include the chemistry in our simulations

- Chemistry sets the thermal state of gas
- It permits to link models and observations
- Different chemical tracers are sensitive to different physical conditions, permiting to probe the medium

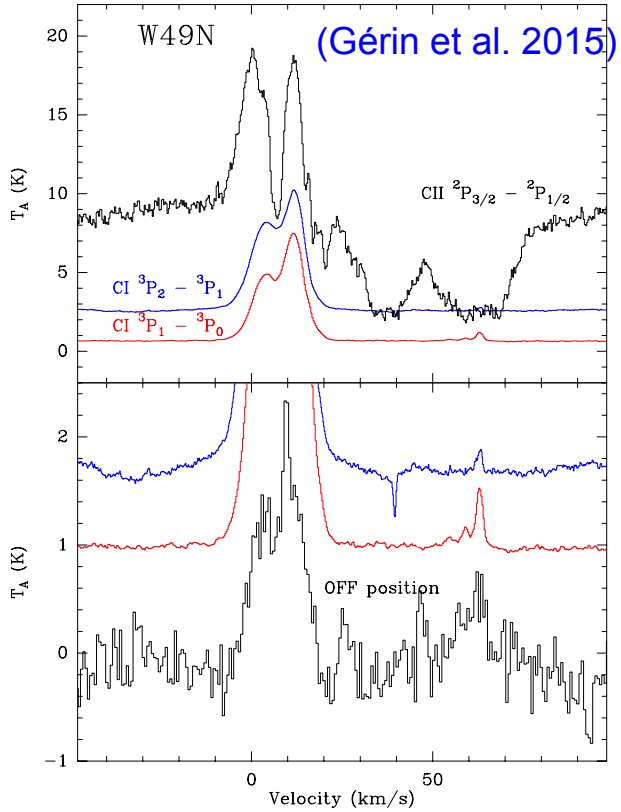
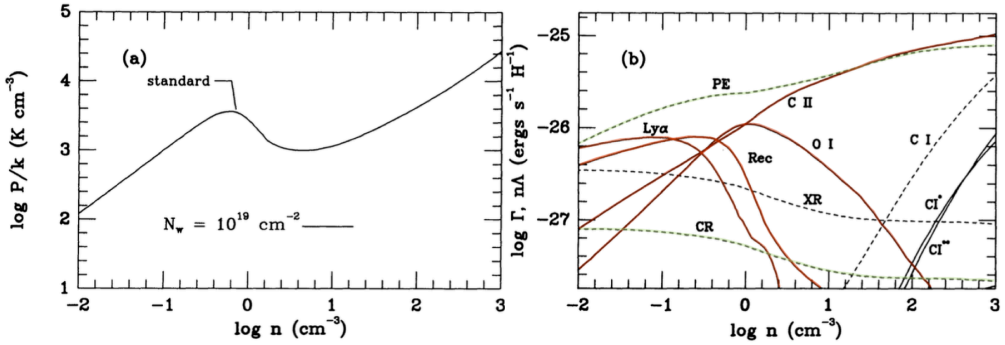


Fig. 1. *Top*: *Herschel*/HIFI spectra towards W49N. The red line shows the [C I]$^3P_1 - {}^3P_0$ line at 492 GHz, the blue line shows the [C I]$^3P_2 - {}^3P_1$ line at 809 GHz and the black line the [C II]$^2P_{3/2} - {}^2P_{1/2}$ line at 1.9 THz. The horizontal axis is the LSR velocity in km s^{-1} and the vertical axis is the SSB antenna temperature in Kelvin. *Bottom*: zoom on the [C I] lines (red, blue as above) and the average [C II] spectrum of the OFF positions (black). The continuum levels have been shifted for clarity in the *bottom panel*.

Why avoid the chemistry in our simulations

- Heating and cooling functions can do the job



(Wolfire et al. 1995)

- Chemistry is computationally demanding:
  - For ~30 species ➡ dt x100 !

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What if we want to make a little effort?

Three possible approaches:

- Full post-processing
- On-the-fly treatment
- Hybrid approaches

On-the-fly chemistry

- In general very reduced chemical networks
  (Glover& Mac Low 2007a,b; Glover & Clark 2012b, Hocuk et al 2015, 2016)
- Species can be advected and diffused within the simulation.
- It can include dynamical effects
- Cooling/heating can be included from the chemistry.
- In general it is extremely slow (~100 times slower for a network of ~30-40 species)
- Further approximations to speed-up the computation:
  Low resolution simulations
  Especially in the radiative transfer and shielding
  (Richings & Schaye 2016)

Full « post-processing » or « at equilibrium » calculations

- Full equilibrium depending on the local physical conditions (ex. PDR codes) (Le Petit et al 2006)
- Exhaustive chemical networks can be used
- Chemistry do not evolve with the gas
- It does not include dynamical effects, or they are imposed artificially (ex. TDR code) (Godard et al 2009, 2014)

Hybrid approaches

- Treat crucial species on-the-fly
- Full equilibrium for the rest of the species
- Chemistry « evolve » with the gas, including dynamical effects

Hybrid approaches:

1. Identify the « crucial species » → H_2
2. Use cooling functions
3. Run your simulation and calculate on-the-fly all crucial species

$$k_{\mathrm{form},0} = 3 \times 10^{-17}\ \mathrm{cm^3\ s^{-1}} \qquad k_{\mathrm{ph},0} = 3.3 \times 10^{-11} G_0\ \mathrm{s^{-1}}$$

$$k_{\mathrm{form}} = k_{\mathrm{form},0} \sqrt{\frac{T}{100\ \mathrm{K}}} \times S(T). \qquad k_{\mathrm{ph}} = \mathrm{e}^{-\tau_{d,1000}} f_{\mathrm{shield}}(\mathcal{N}_{\mathrm{H_2}}) k_{\mathrm{ph},0}.$$

4. Calculate the chemical abundances in post-processing, following the evolution of the crucial species using a chemical solver. →

Hybrid approaches: Solver

- Adapted from the Meudon PDR code (Le Petit et al. 2006)
- The equation system is solved using a Newton-Raphson

149 species
2694 equations

- H2 fix → Fix HI

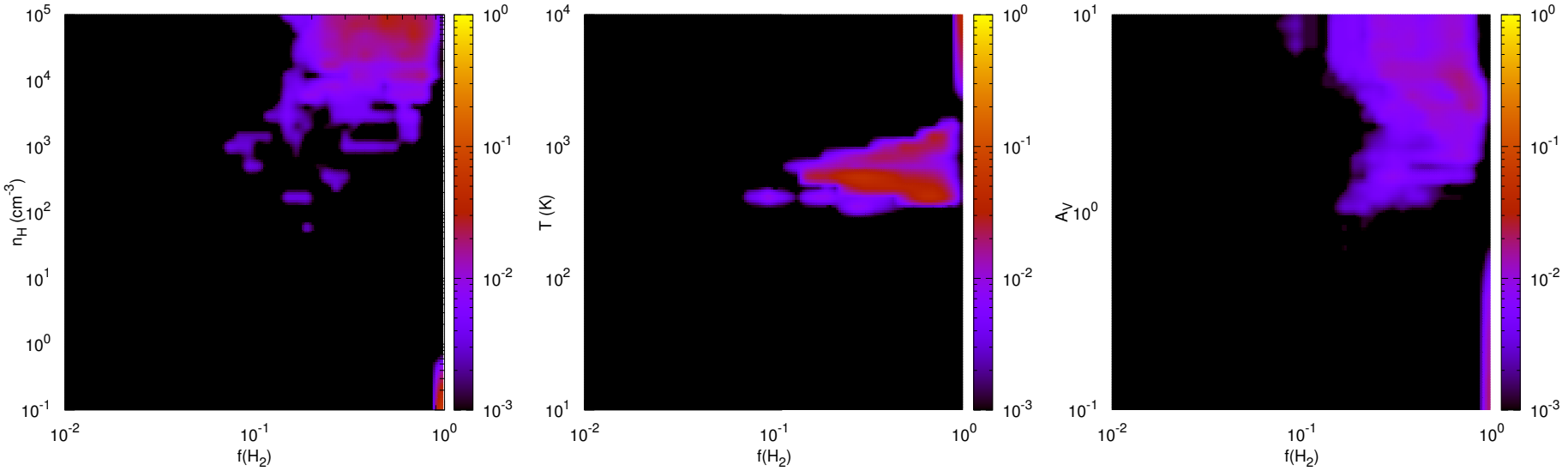
Parameters of the chemical solver

mandatory			
χ	mathis	1	external UV radiation field
A_V	mag	0 – 3	visible extinction
T_K	K	$10 - 10^4$	kinetic temperature
$n_{\rm H}$	$\rm cm^{-3}$	$10 - 10^4$	gas density
$\zeta_{\rm H_2}$	$\rm s^{-1}$	10^{-16}	CR ionisation rate of H_2
optional			
$f_{\rm sh,\ H_2}$		$10^{-3} - 1$	H_2 self-shielding factor[a]
$f_{\rm sh,\ CO}$		$10^{-3} - 1$	CO self-shielding factor[a]
$x(\rm H_2)$		$10^{-3} - 1$	H_2 abundance
v_d	$\rm km\ s^{-1}$	$10^{-3} - 20$	ion-neutral velocity drift

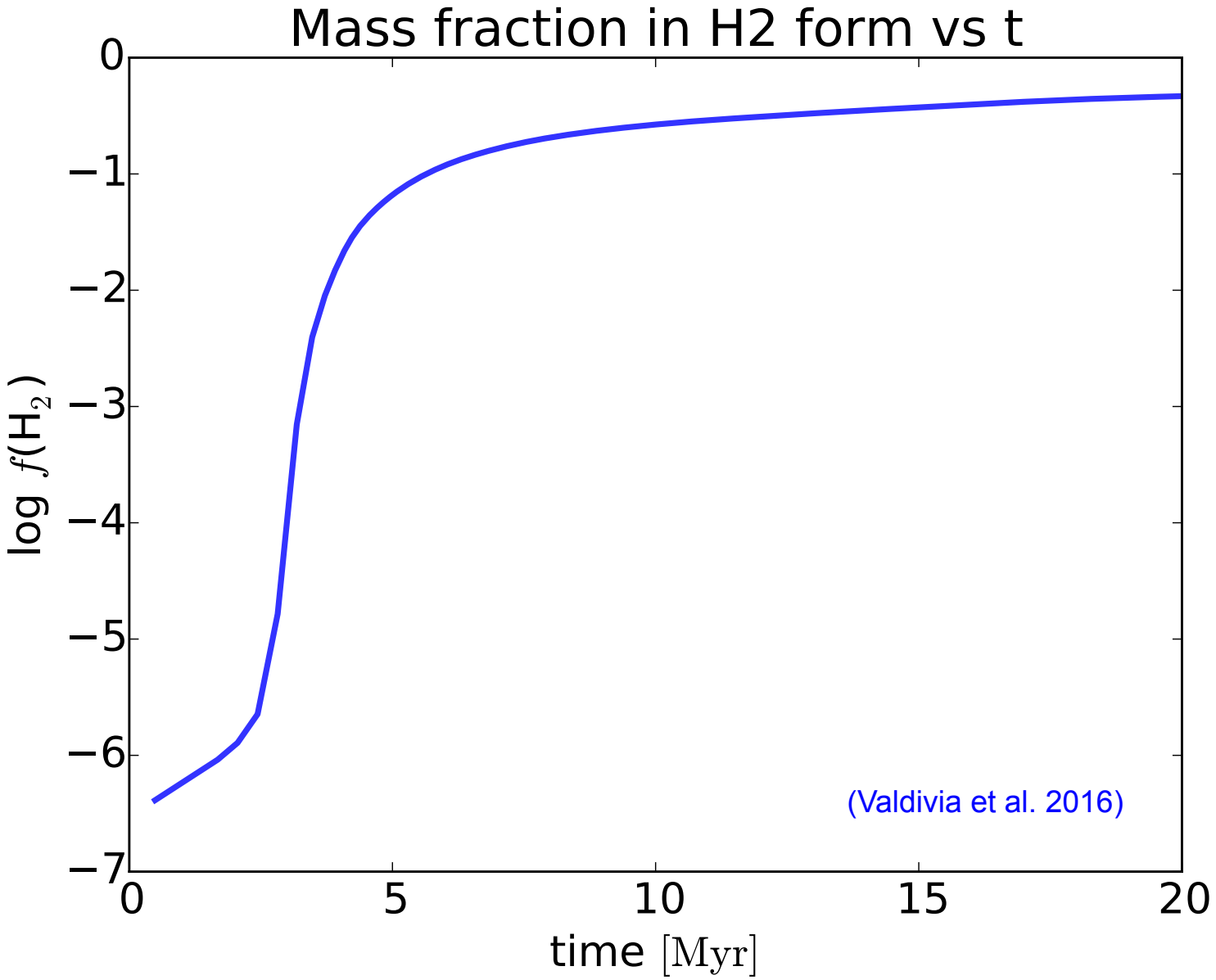
(*a*) Valdivia et al. (2016)

Hybrid approaches: Solver performance

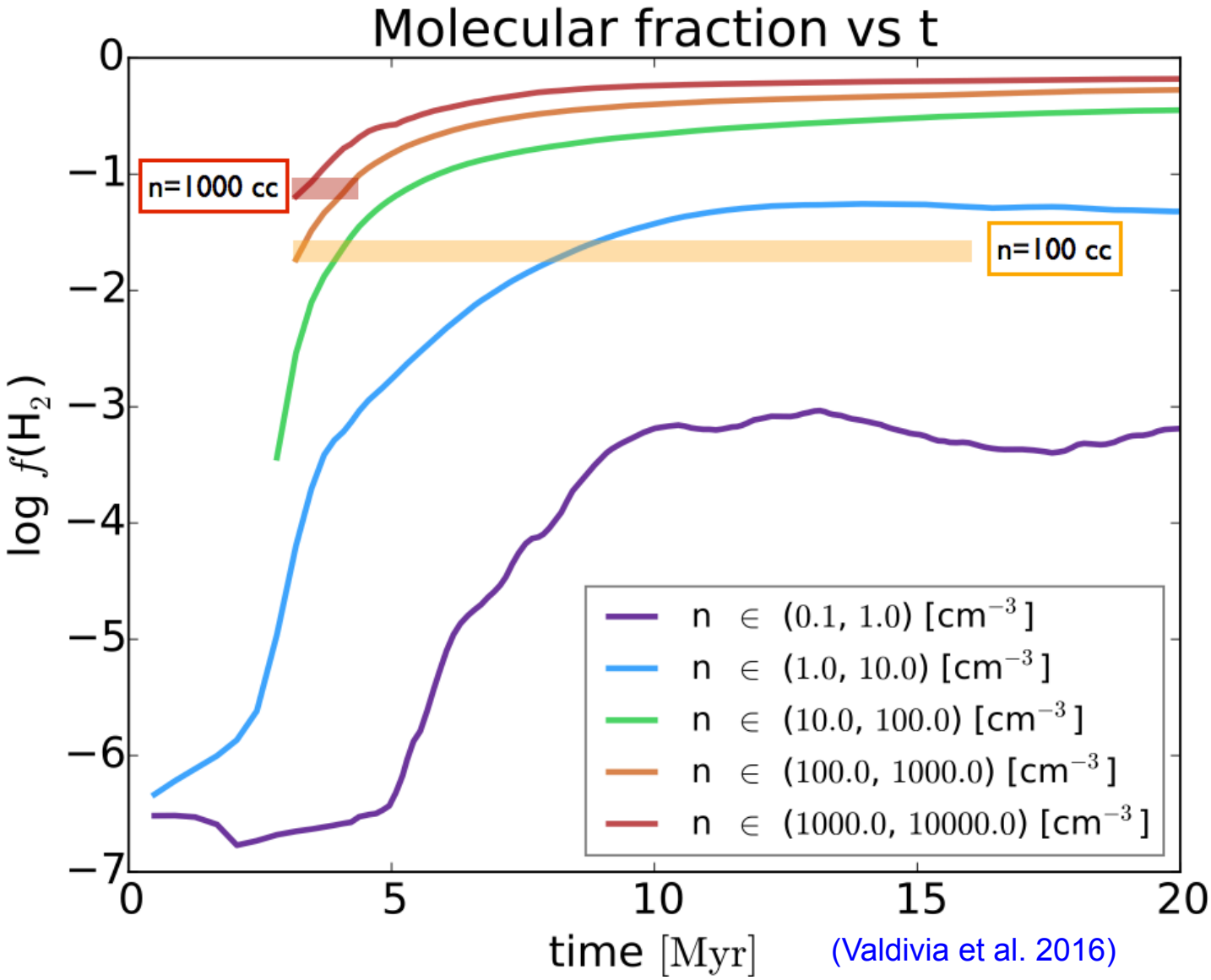
- Some limitations: Fixing a species can prevent the existence of a solution at equilibrium, or it can be difficult to reach it.



Some results on-the-fly

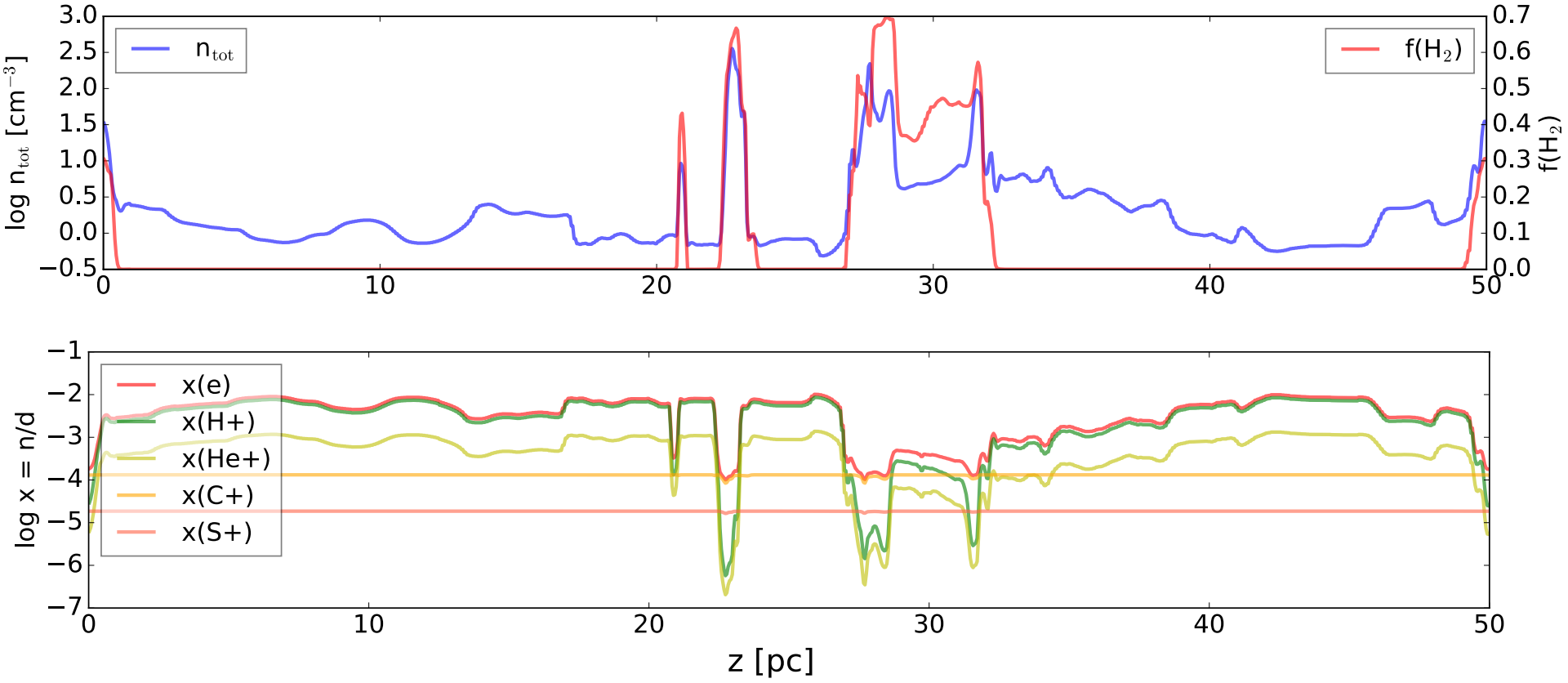


Some results on-the-fly



(Valdivia et al. 2016)

Some results post-processing



(Valdivia et al. 2016b, in prep.)

Conclusions (or take home messages)

- 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.
- Fixing a species can prevent the existence of a solution at equilibrium.
- Some species appear very late, but when they do it they can survive a long time and advection terms can play an important role.

(J. Howard Miller 1943)

For more physical results:

« Consequences of warm H2 on the chemistry of diffuse molecular clouds: the case of CH+ » (S08, Friday)