

A sub-grid model for molecular gas in a cosmological galaxy formation simulation

- MASTERS' THESIS DEFENCE -

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The space between stars

- Till mid-1960's - interstellar space too hostile for the existence of appreciable quantities of molecules.
- Early 1970's - fragile molecules were observed (NH_3 , H_2O , H_2CO , etc.)
- Observations led to the onset of rigorous studies and modelling of chemistry in the interstellar medium (ISM).

Interstellar Medium (ISM)

- ISM - the space between stars is filled with gas and dust
- Generally, low densities and low temperatures
- But extreme regions with large variations in density and temperature also exist

GMC - Formation

- Interstellar space - filled with UV radiation from stars
- This background radiation is responsible for breaking apart molecules into atoms, a process known as photo-dissociation.
- These photons are usually in the Lyman-Werner (LW) energy band: 11-13.6 eV

GMC - Formation

- Interstellar space also contains significant amounts of dust
- Dust is capable of blocking out starlight.
- Dust accumulation - a region in which the UV radiation from stars is blocked.
- This allows for the formation of molecules such as H_2 , CO , H_2O , NH_3 , CH , CN , etc.

GMC - Formation

- These molecules begin to accumulate - gravity pulls all the gas together to form large gas structures known as *Giant Molecular clouds (GMCs)*.
- Average density within these clouds : 10^2 - 10^3 [H]/cc - much denser than the surrounding interstellar space.
- High density - molecular clouds block UV starlight - the typical temperature of molecular gas clouds: 10 K
- Size ~ 100pc across, Mass ~ $1-2 \times 10^5$ solar masses

GMC - Characteristics

- The density within these clouds is not uniform.
- The region with higher density, where lots of dust and gas cores reside, are called *clumps*.
- If the gravity in these clumps is able to overcome the high density, and forces the dust and gas to collapse, then these clumps will begin to form stars.
- The process of formation of these clumps in the cloud is called fragmentation.

GMC - Observation

- A good way to study the characteristics of a GMC - emission and absorption spectra of its constituent atoms and molecules.
- The most abundant molecule in these clouds is molecular hydrogen (H_2). But H_2 lacks an electric dipole - first quadruple line excitation temperature ($T_{exc} \approx 500K$) is much higher than the kinetic temperature of the surrounding molecular cloud ($T_K \approx 10K$).
- Not possible to observe H_2 - it does not radiate or absorb even at radio wavelengths.

GMC - Observation

- Carbon monoxide (CO) - 2nd most abundant molecule in GMC
- For CO , $T_{exc} \approx 5K$,i.e., CO is easily excited inside the molecular cloud.
- Since CO tends to be present wherever H_2 is found, the frequencies emitted from CO molecules and the strength of the corresponding spectral lines enable astronomers to infer the H_2 density in the emitting region.

Line Transfer

- Gas in the GMC can be studied - emission and absorption spectra of the gas molecules.
- The gas atoms or molecules have discrete energy states.
- Atom or molecule jumps from one energy state to another - bound-bound transitions.
- Two types: collisional transitions and radiative transitions.

Line Transfer - Energy levels & occupation numbers

- The total number of energy states/levels of an atom or molecule = N_{levels}
- If, $i = 1, 2, \dots, N_{levels}$, then energy of each level is denoted as E_i , and in ascending order of energies the order is : $E_{i+1} \geq E_i$.
- n = total number density of atoms or molecules per cc, and n_i = the occupation number density belonging to each level, then,
Fractional occupation number x_i is then defined as: $x_i = \frac{n_i}{n}$

Line Transfer - Energy levels & occupation numbers

- Collisions between atoms or molecules can cause the atom/molecule to transit from any state i to other state j .
- When density is high, these collisions take place so often that it can be assumed that x_i are thermally distributed, i.e.,

$$\frac{x_j}{x_i} = \frac{n_j}{n_i} = \frac{g_j}{g_i} e^{-\left(E_j - E_i\right)/k_B T}$$

$$Z(T) = \sum_i g_i e^{-(E_i - E_j)/k_B T}$$

$$x_i = \frac{1}{Z(T)} g_i e^{-(E_i - E_j)/k_B T}$$

Line transfer - Emission & absorption coefficients

- If an atom or molecule jumps from one energy level to another by absorbing or emitting a photon, the transition is called a radiative transition, or a spectral line transition.
- This means that the radiative transfer equation has to be solved :

$$\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu$$

where j_ν is the emissivity coefficient, and α_ν is the absorption coefficient.

Line transfer - Emission & absorption coefficients

- For two levels i and j , such that $E_i > E_j$, the energy difference between the levels is given by:

$$h\nu_{ij} = E_i - E_j$$

- For pure line emission, the emissivity coefficient j_ν is given as:

$$j_\nu = \frac{h\nu_{ij}}{4\pi} n_i A_{ij} \phi_{ij}(\nu)$$

- Similarly, the absorption coefficient α_ν :

$$\alpha_\nu = \frac{h\nu_{ij}}{4\pi} \left(n_j B_{ji} - n_i B_{ij} \right) \phi_{ij}(\nu)$$

Line transfer - Line Profile Function

- The line profile function is written here as a Gaussian :

$$\phi_{ij}(\nu) = \frac{1}{\left(2\pi\Delta\nu_{ij}^2\right)^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{\nu - \nu_{ij}}{\Delta\nu_{ij}}\right)^2\right]$$

where $\Delta\nu_{ij}$ is the line width in Hz.

- There can be different models for the computation of the line width $\Delta\nu_{ij}$

Line transfer - Line Profile Function

- The simplest model is the thermal line broadening.
- In this case the line broadening is caused by the thermal motion of the gas particles, i.e., $\Delta\nu_{ij} = \nu_{ij} \frac{c_s}{c}$, where $c_s = \sqrt{\frac{k_B T}{m}}$ is the isothermal sound speed of the atomic or molecular species at $T = \bar{T} = 10\text{K}$, and m is the mass of the species.

Line transfer - Line Profile Function

- Another source of randomised line broadening can be micro-turbulence or sub-grid turbulence.
- Sub-grid turbulence is the turbulence on the spatial scales smaller than the smallest grid size. This small-scale turbulence must be treated as a velocity dispersion.

$$\Delta\nu_{ij} = \nu_{ij} \frac{\Delta v}{c}$$

- where Δv is the turbulent velocity dispersion in the volume element under

consideration, such that: $\Delta v = \sqrt{\frac{1}{3} \langle v_{\text{turb}}^2 \rangle_{3D}}$

Line transfer - Optical depth & escape probability

- In line transfer energy (or photons) can be transported via the lines.
- But if the optical depth is very large in all the lines that are appreciably emitting light, then the transport of the energy is hampered substantially.
- It is then useful to look at the various ways by which radiation can nevertheless escape.

Line transfer - Optical depth & escape probability

- The Sobolev approximation computes the optical depth τ_{ij} as:

$$\tau_{ij} = \frac{h\nu_{ij} n L}{4\pi\sqrt{2\pi}\Delta\nu_{ij}}(x_j B_{ji} - x_i B_{ij})$$

- The probability of a photon to escape from a cloud:

$$\beta_{ij} = \frac{1 - e^{-\tau_{ij}}}{\tau_{ij}}$$

Different scales in the model

Three scales/regimes in the model:

- Macroscopic length scale - a cloud or a clump.
- Microscopic length scale - particles inside the volume element
- Mesoscopic scale - between the macroscopic and microscopic scales, and are usually unresolved

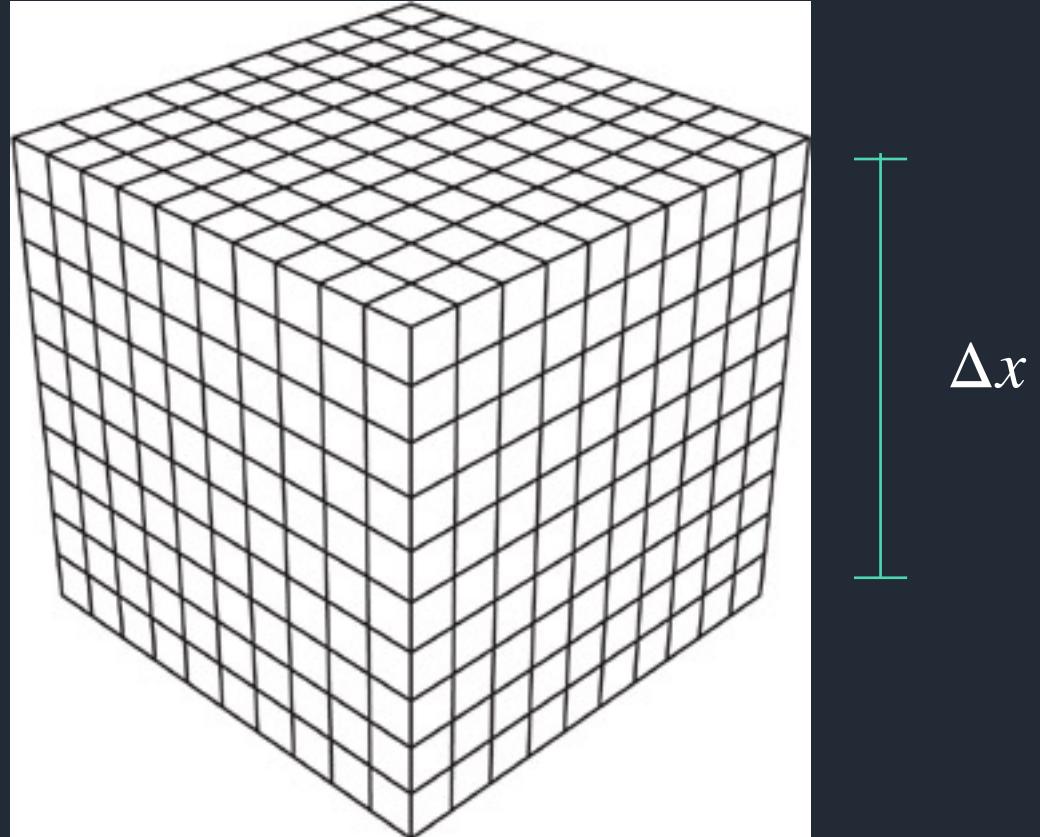
Different scales in the model

$$\Delta v(\ell_s) = \Delta v \sqrt{\frac{\ell_s}{\Delta x}}$$

$$\Delta v(\ell_s) = c_s$$

$$\ell_s = \frac{\Delta x}{\mathcal{M}^2}$$

ℓ_s 



Density field of the sub-grid model

The density field of an isothermal, non-gravitating, turbulent gas is well described by a log-normal Probability Distribution Function (PDF).

$$P_V(s) = \frac{1}{(2\pi\sigma_s^2)^{1/2}} \exp \left[-\frac{1}{2} \left(\frac{s - \bar{s}}{\sigma_s} \right)^2 \right]$$

$$\bar{s} = -\sigma_s^2/2$$

$$s = \ln \left(n_H / \bar{n}_H \right)$$

$$\sigma_s^2 = \ln \left(1 + b^2 \mathcal{M}^2 \right)$$

Length scale of the absorbing layer

- Gaussian PDF: describes the density for the sonic length volume elements inside a macroscopic cell.
- Jeans length: the length scale of the absorber for these density fluctuations.

$$\lambda_J = \frac{c_s}{\sqrt{4\pi G n_H m_p}}$$

$$c_s = \sqrt{\frac{k_B T}{m_p}}$$

$$T = \bar{T} = 10\text{K}$$

Length scale of the absorbing layer

- Volume elements with size $>$ Jeans length: no collapse, either stay like that or diffuse away
- Volume elements with size $<$ Jeans length: collapse and disappear
- Volume elements with size \sim Jeans length: onset of collapse, emerging out of the density fluctuations

$$\lambda_J = \frac{c_s}{\sqrt{4\pi G n_H m_p}}$$

$$c_s = \sqrt{\frac{k_B T}{m_p}}$$

$$T = \bar{T} = 10\text{K}$$

Power-law PDF due to self-gravity

- Self-gravity : more and more denser clumps start to form
- This increase in probability of finding denser clumps results in developing a power-law tail on the high-density side of the PDF.
- Confirmed by recent observations

Power-law PDF due to self-gravity

- Power-law PDF model: based on the formalism of free-fall spherical collapse

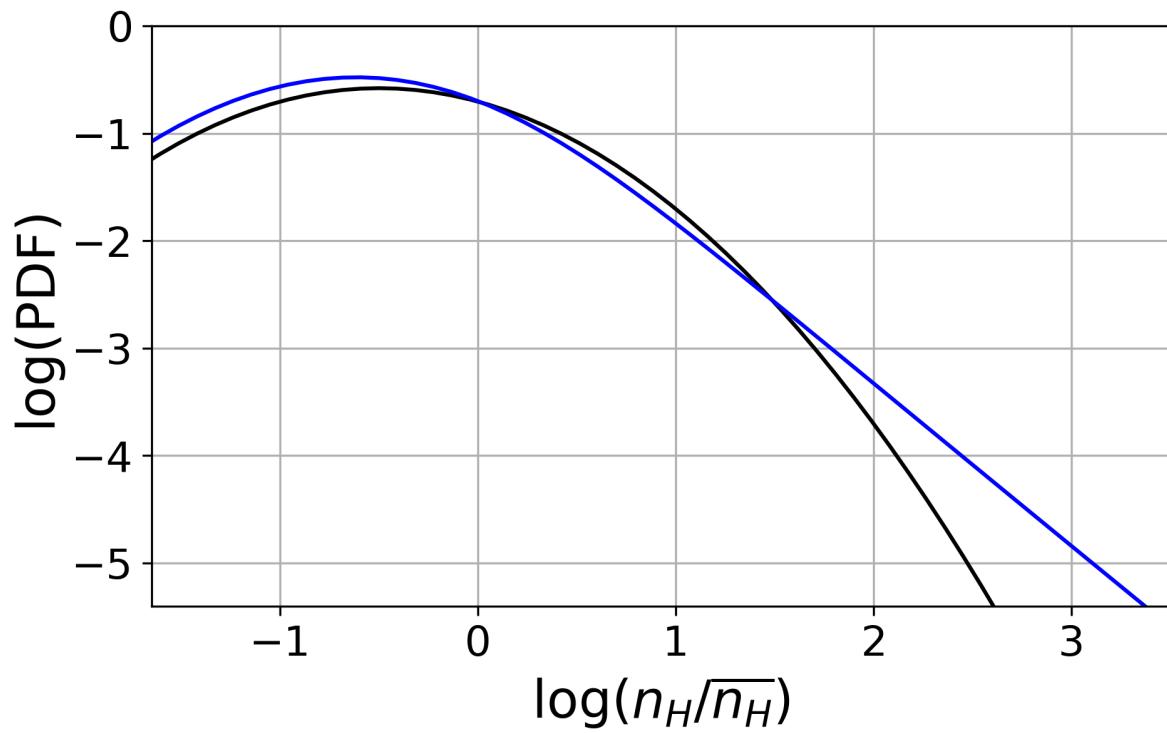
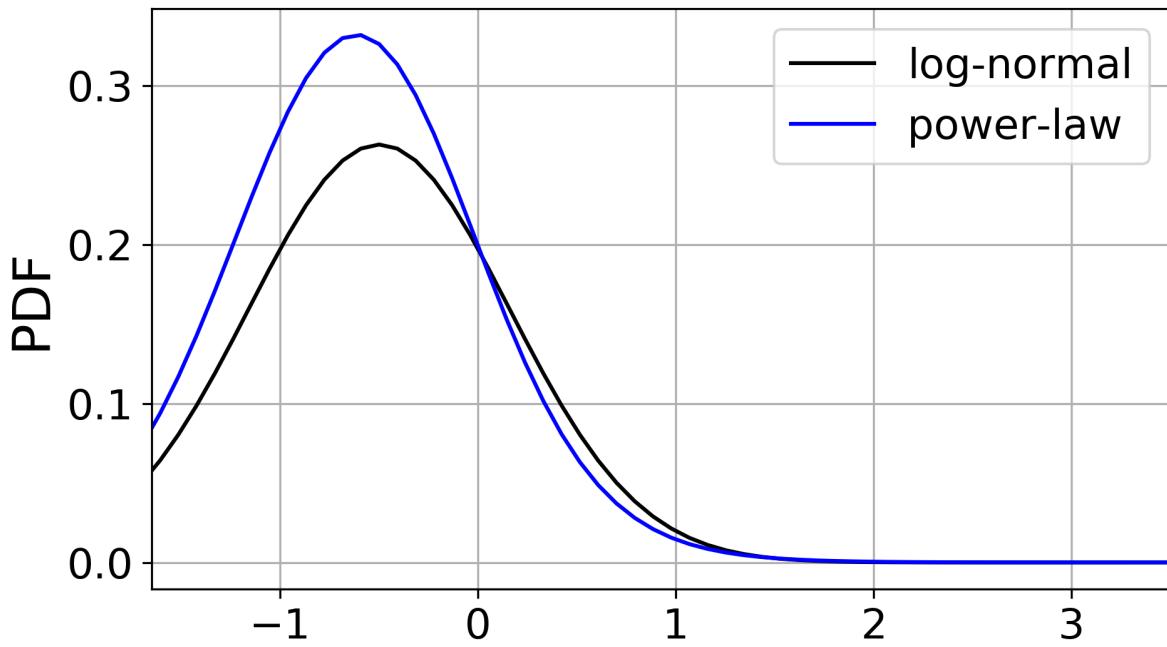
$P_V(s, t)$ = functional form of the PDF at any given time

$P_V(s, 0) \equiv P_V(s)$, the initial PDF described as the log-normal PDF

$$n_H = \frac{n'_H}{\left[1 - \left(\frac{t}{t_{ff}}\right)^2\right]^2}$$

$$t_{ff} = \sqrt{\frac{3\pi}{32 G n'_H}}$$

$$P_V(s) = \frac{P'_V(s)}{\int \exp(s) P'_V(s) ds}$$



H₂ formation model

- Creation rate of H₂ molecules:

$$CR = k \ Z \ n_{\text{HI}} \ n_H$$

- Destruction rate of H₂ molecules:

$$DR = c \ \sigma_{\text{dust}} \ n_{\text{H2}} \ n_{\text{LW}}$$

- Relation between number density of H atoms and H₂ molecules:

$$n_H = n_{\text{HI}} + 2n_{\text{H2}}$$

H₂ formation model

Solving for equilibrium conditions:

$$n_H = \left(\frac{c \sigma_{\text{dust}} n_{\text{H}2} n_{\text{LW}}}{k Z n_H} + 2 \right) n_{\text{H}2}$$

Molecular fraction of H₂:

$$X_{\text{H}2} = \frac{n_{\text{H}2}}{n_H} = \frac{1}{2 + \left(\frac{c \sigma_{\text{dust}} n_{\text{H}2} n_{\text{LW}}}{k Z n_H} \right)}$$

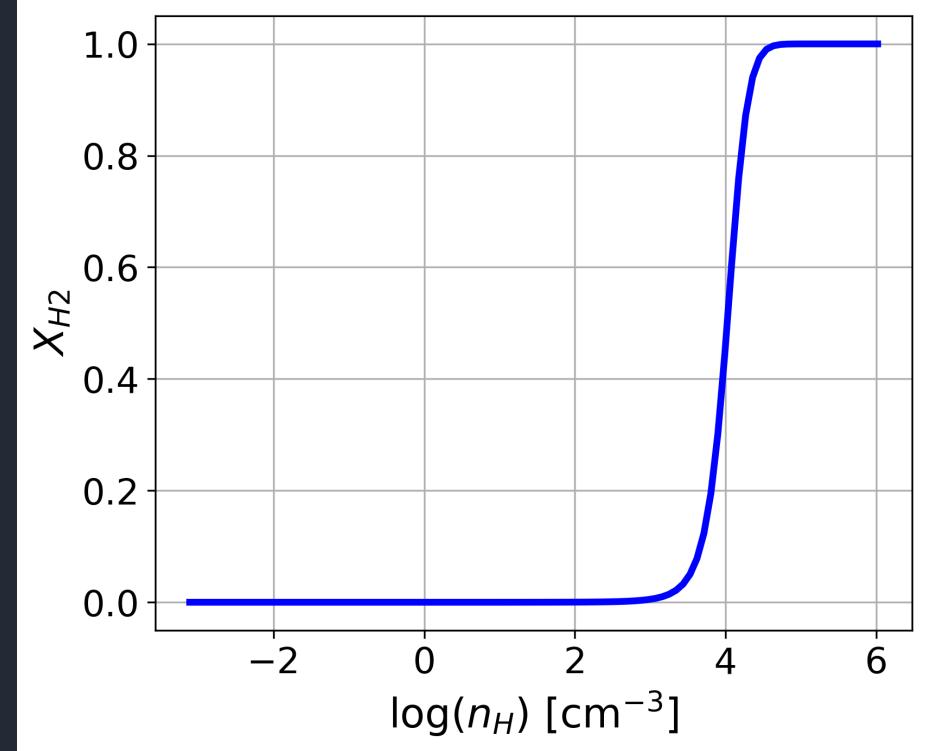
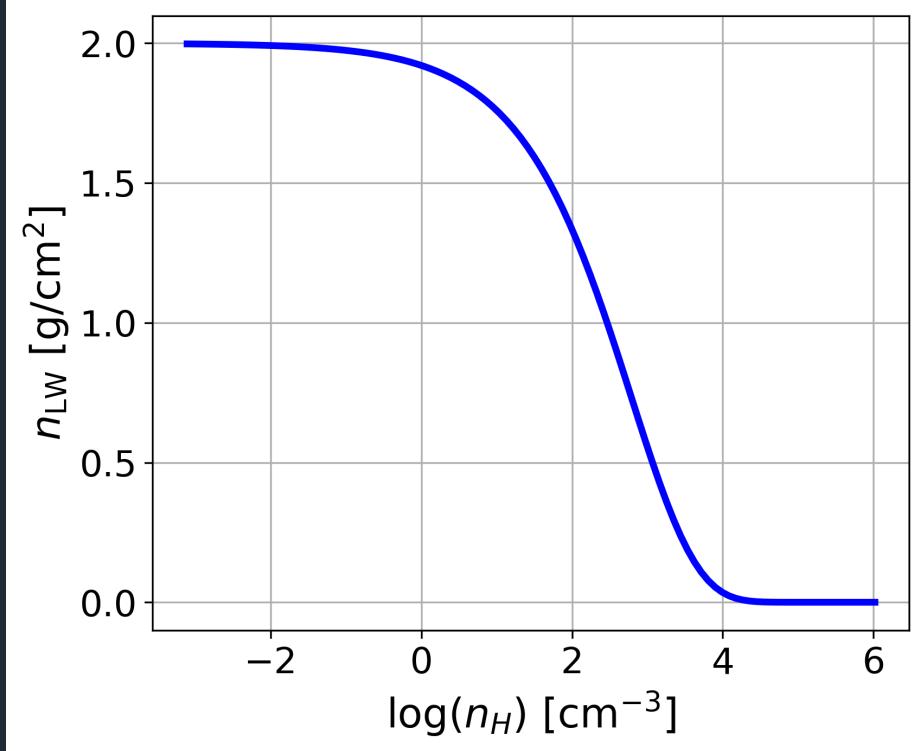
Number of photo-dissociating Lyman-Werner (LW) photons:

$$n_{\text{LW}} = (\text{ISRF}) e^{-\tau_{\text{LW}}} = G e^{-\tau_{\text{LW}}}$$

The optical depth in the Lyman-Werner (LW) band due to dust:

$$\tau_{\text{LW}} = 1000 m_p Z n_H \lambda_J$$

Plot:



Self-shielding of H₂

$$S_{H_2} = \frac{0.965}{(1 + x/b_5)^2} + \frac{0.035}{\sqrt{1 + x}} \exp\left(-\frac{\sqrt{1 + x}}{1180}\right)$$

$$x \equiv N_{H_2}/5 \times 10^{14} \text{cm}^{-2}$$

$N_{H_2} = n_{H_2} \lambda_J$ = Column density of H_2

$$b_5 \equiv b_0/\text{km/s}$$

$$b_0 = \sqrt{2} \Delta v(\lambda_J)$$

Self-shielding of H₂

- Number of photo-dissociating Lyman-Werner (LW) photons:

$$n_{\text{LW,SS}} = G_0 \ S_{H_2} \exp(-\tau_{\text{LW}})$$

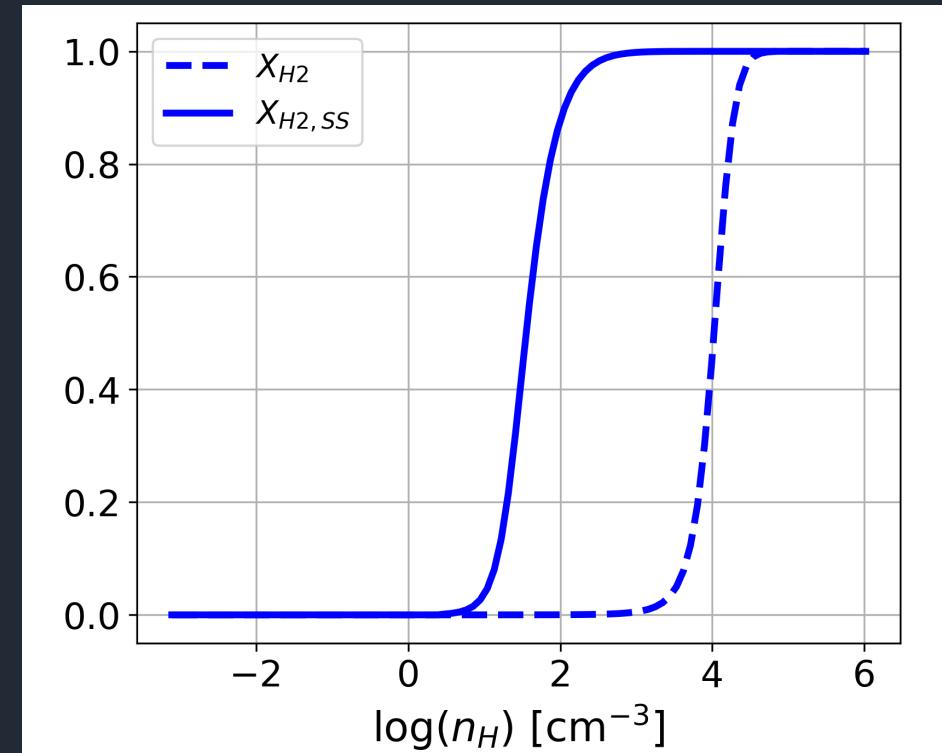
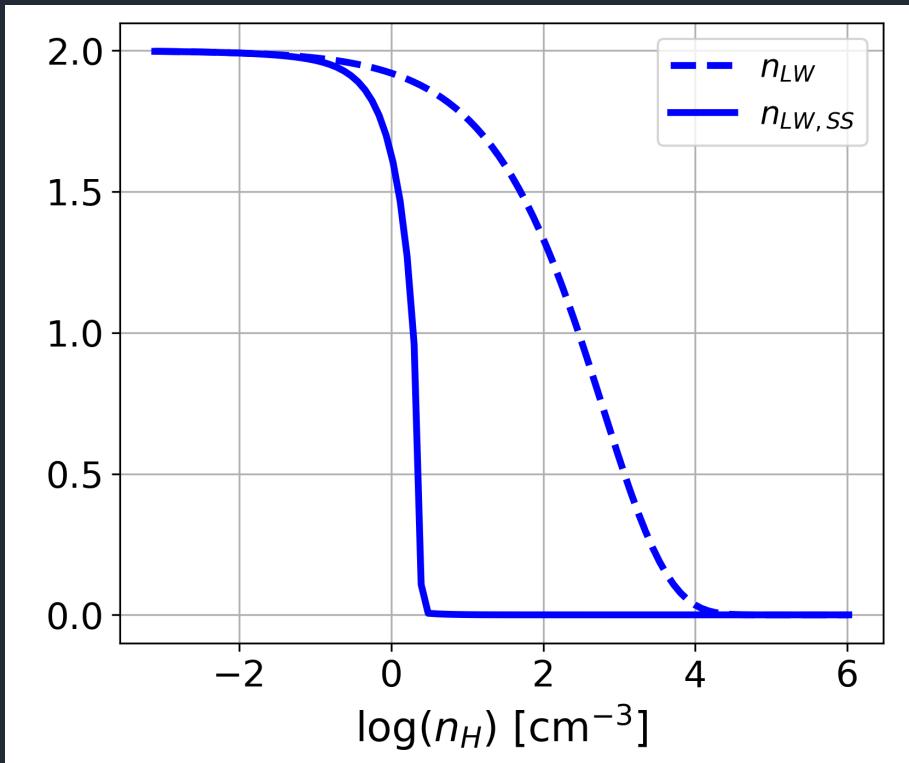
- Molecular fraction of H₂:

$$X_{H_2,\text{SS}} = \frac{1}{2 + \left(\frac{c \ \sigma_{\text{dust}} \ n_{H_2} \ n_{\text{LW,SS}}}{k \ Z \ n_H} \right)}$$

- Number density of H₂ molecules:

$$n_{H_2,\text{SS}} = n_H \ X_{H_2,\text{SS}}$$

Plot:



CO formation model

- CO formation model is similar to the H₂ formation model.

- Molecular fraction of CO:

$$X_{CO} = \frac{1}{1 + \frac{\Gamma_{CO}}{n_{H2} k_0 \zeta}}$$

- Number density of CO molecules:

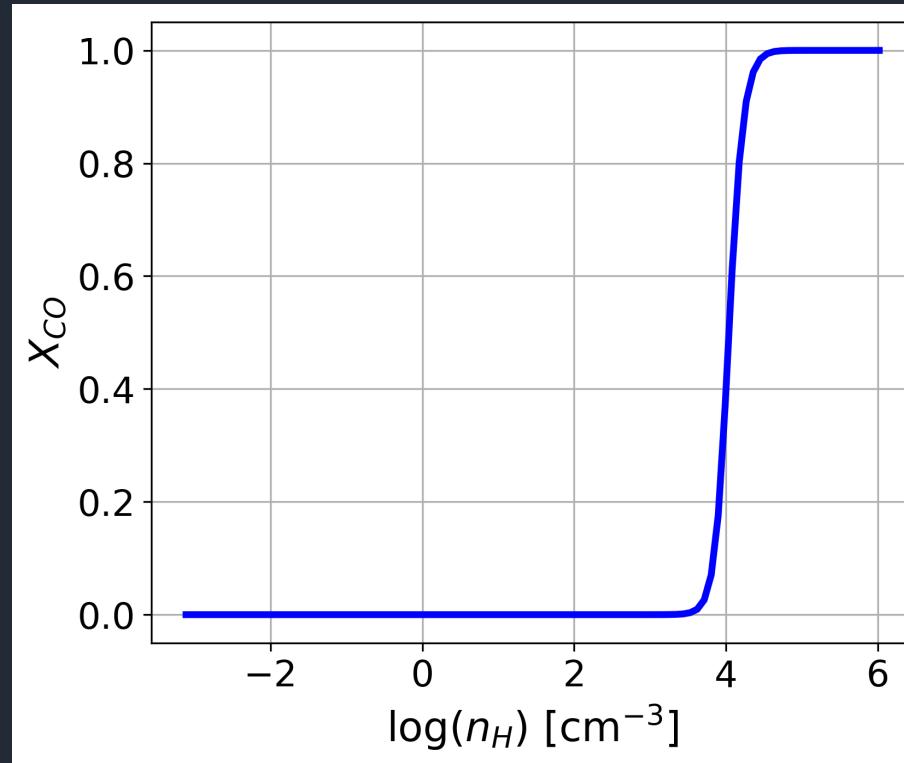
$$n_{CO} = 10^4 \times Z n_H X_{CO}$$

$$\zeta = \left[1 + \frac{\Gamma_{CH_X}}{n_H k_1 x_O} \right]^{-1}$$

$$\Gamma_{CO} = 10^{-10} n_{LW}$$

$$\Gamma_{CH_X} = 5 \times 10^{-10} n_{LW}$$

Plot:



Line radiative transfer

- A simplified routine for line radiative transfer: LTE-only
- For CO:

N_{tot} = the total number of energy levels

E_i , g_i = Energy and statistical weight of each level

ν_{ij} = frequencies of transitions between different energy levels

A_{ij} = the Einstein-A coefficient

B_{ij} B_{ji} = Einstein-B coefficients calculated using Einstein relations

Leiden Atomic
and Molecular
Database
(LAMDA) file

Line radiative transfer

- For CO:

Using N_{tot} , E_i , and g_i from the LAMDA file

And using $T = \bar{T} = 10\text{K}$

Partition function (Z)
& fractional occupation number (x_i)
are computed.

- In this model, only the first CO transition is considered, i.e., the transition from the first excited state to the ground state, i.e.,

$$i = 1$$

$$j = 0$$

Also, $n \equiv n_{CO}$

Line radiative transfer

- The integrated emissivity of CO(1-0) transition line:

$$j_{10} = h\nu_{10} n_{CO} x_1 A_{10}$$

- Luminosity density of the CO(1-0) transition line:

$$\ell_{CO} = j_{10} \beta_{10}$$

Line radiative transfer

- UNITS:

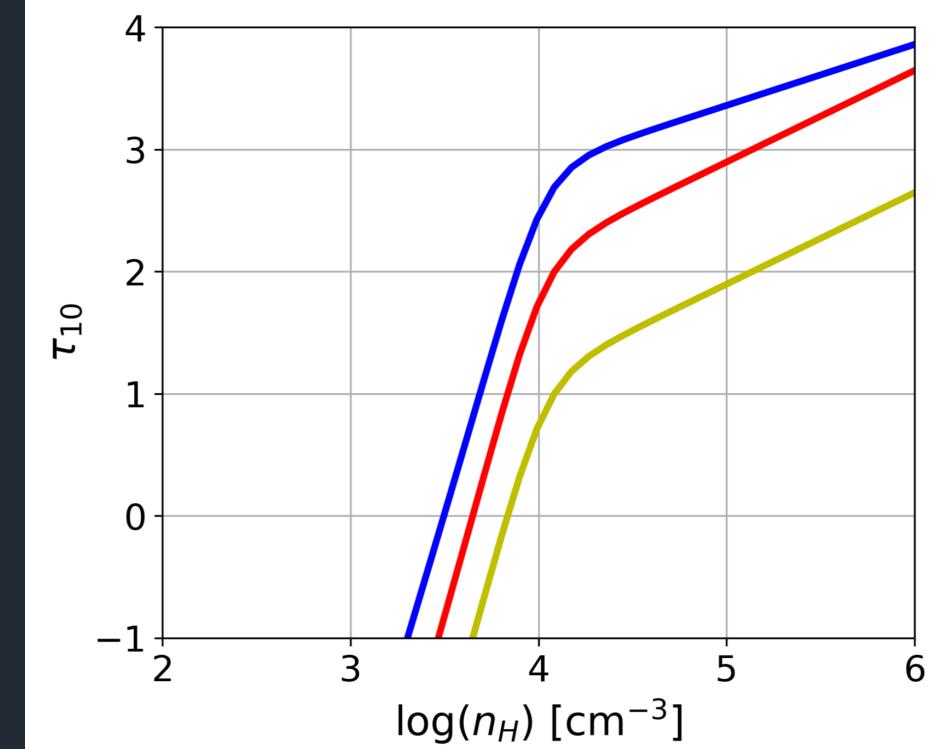
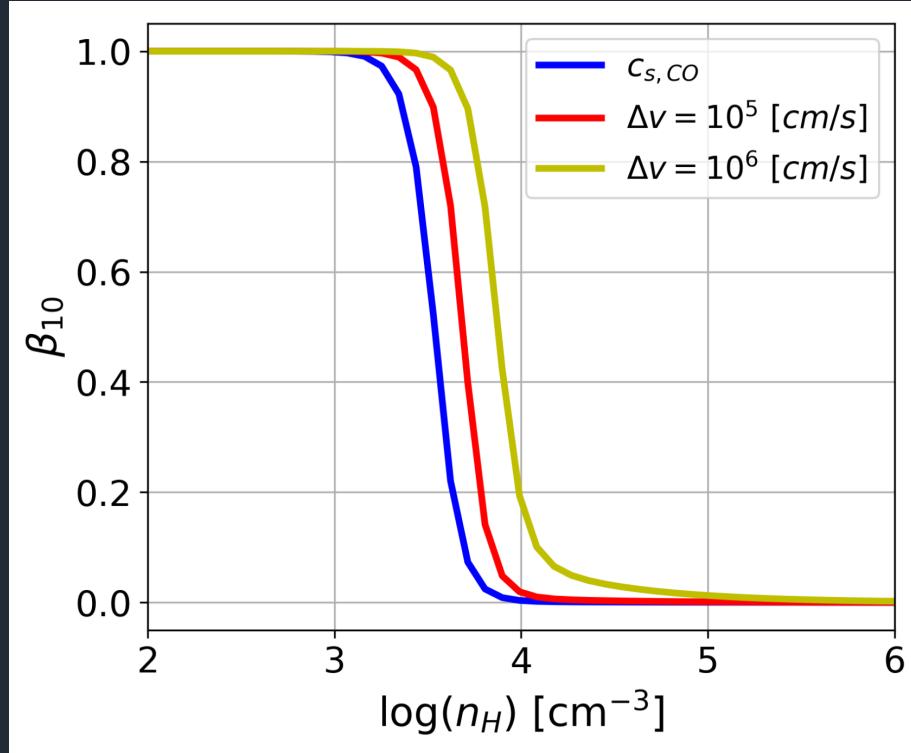
$$\ell_{CO} \text{ [K km s}^{-1}\text{pc}^2\text{cm}^{-3}] = \frac{1}{2k_B} \left(\frac{c}{\nu} \right)^3 \ell_{CO} \text{ [erg s}^{-1}\text{cm}^{-3}]$$

- Also, the ratio between the luminosity density and the total gas density: ($\beta_{10} = 1$)

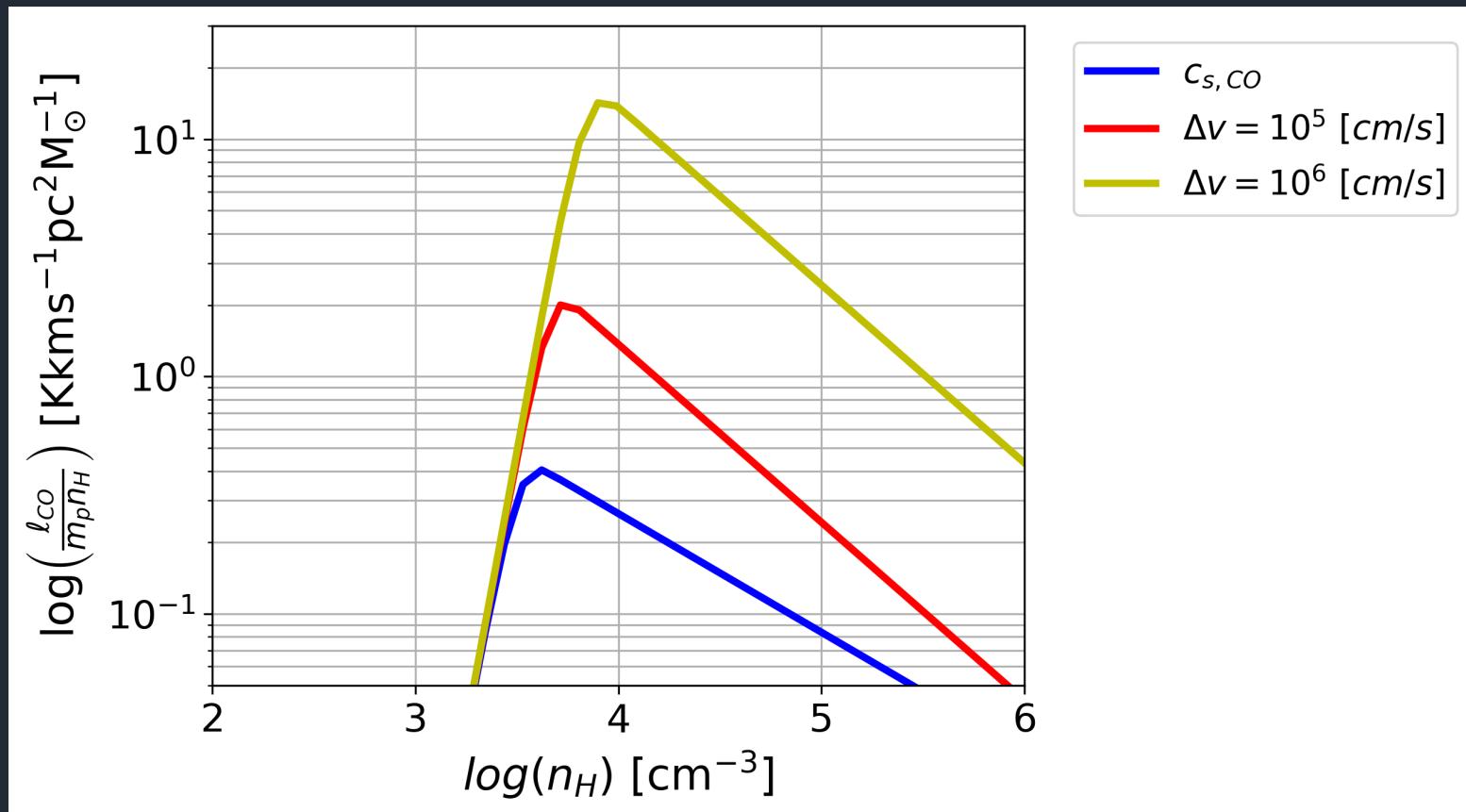
$$\frac{\ell_{CO}}{n_H m_p} = h\nu_{10} \times 10^{-4} \times \frac{Z}{Z_\odot} \frac{x_1 A_{10}}{m_p} \quad n_{CO} = 10^{-4} \times \frac{Z}{Z_\odot} n_H$$

$$\frac{\ell_{CO}}{n_H m_p} = 0.00143 \text{ [erg s}^{-1}\text{g}^{-1}] = 191.383 \text{ [K km s}^{-1}\text{pc}^2\text{M}_\odot^{-1}]$$

Plot:



Plot:



Salient features of the simulation

- The galaxy selected is from an N-body simulation with 512^3 particles in a box size $25h^{-1}\text{Mpc}$

$$z \approx 0.6$$

$$M_{\text{gas}} = 1.3 \times 10^{10} \text{M}_\odot$$

$$R_{vir} \sim 150 \text{kpc}$$

$$M_\star = 1.8 \times 10^{10} \text{M}_\odot$$

$$0.1 \times R_{vir}$$

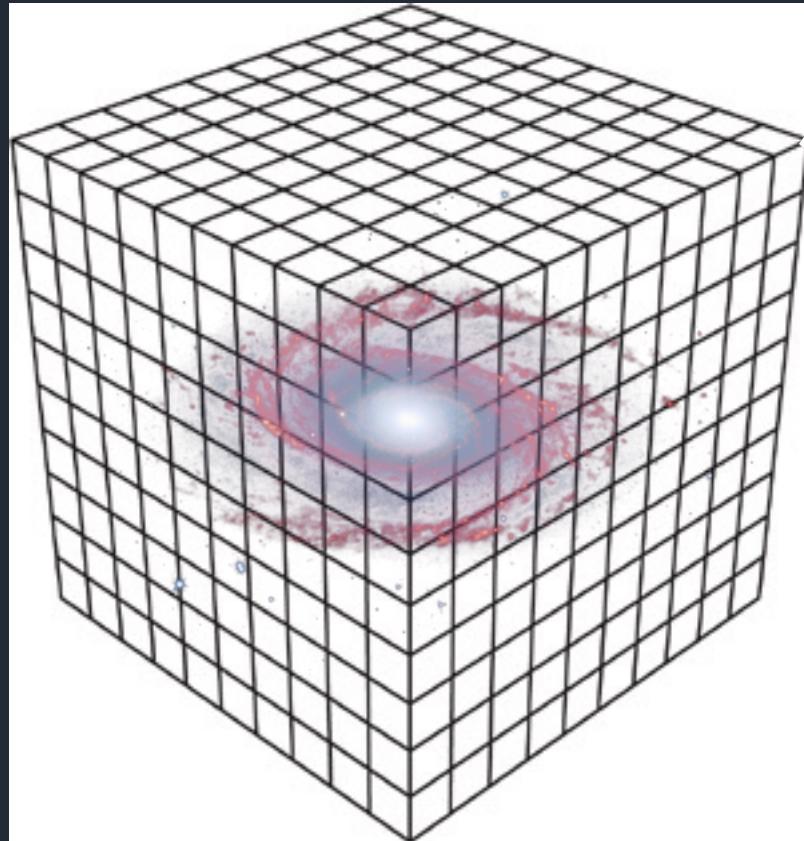
$$\text{SFR} \approx 2 \text{M}_\odot \text{yr}^{-1}$$

$$M_{vir} = 7.9 \times 10^{11} \text{M}_\odot$$

$$l_{max} = 19 \quad \Delta x_{min} \sim 80 \text{pc}$$

Salient features of the simulation

- The simulation is based on the Adaptive Mesh Refinement (AMR) code RAMSES
- AMR technique - computational space is divided into smaller cubical cells.
- The size of each of these simulation cells can be constrained individually on the basis of a parameter of choice.
- This allows to adaptively refine the spatial resolution and lower the computation time.



Galaxy Simulation

For each cell in this simulation → SUB-GRID MODEL

For each of these simulation cells,
the macroscopic parameters are:

$$Z \quad \overline{n_H} \quad T \quad \Delta v \quad \Delta x \quad \mathcal{M} = \frac{\Delta v}{c_s}$$

Applying the sub-grid model on
each simulation cell to compute:

$$\overline{X_{H_2}}$$

$$\overline{X_{CO}}$$

$$\overline{\ell_{CO}}$$

Applying the model on the simulation

$$\overline{X_{H_2}} = \int X_{H_2,ss}(s) \exp(s) P_V(s) ds$$

$$\overline{X_{CO}} = \int X_{CO}(s) \exp(s) P_V(s) ds$$

$$\overline{\ell_{CO}} = \int \ell_{CO}(s) P_V(s) ds$$

$$s = \ln \left(\frac{n_H}{\bar{n}_H} \right)$$

Applying the model on the simulation

- The total luminosity of the galaxy:

$$L_{CO} = \sum_{cells} (\overline{\ell}_{CO}) (\Delta x)^3$$

- The total H₂ mass in the galaxy:

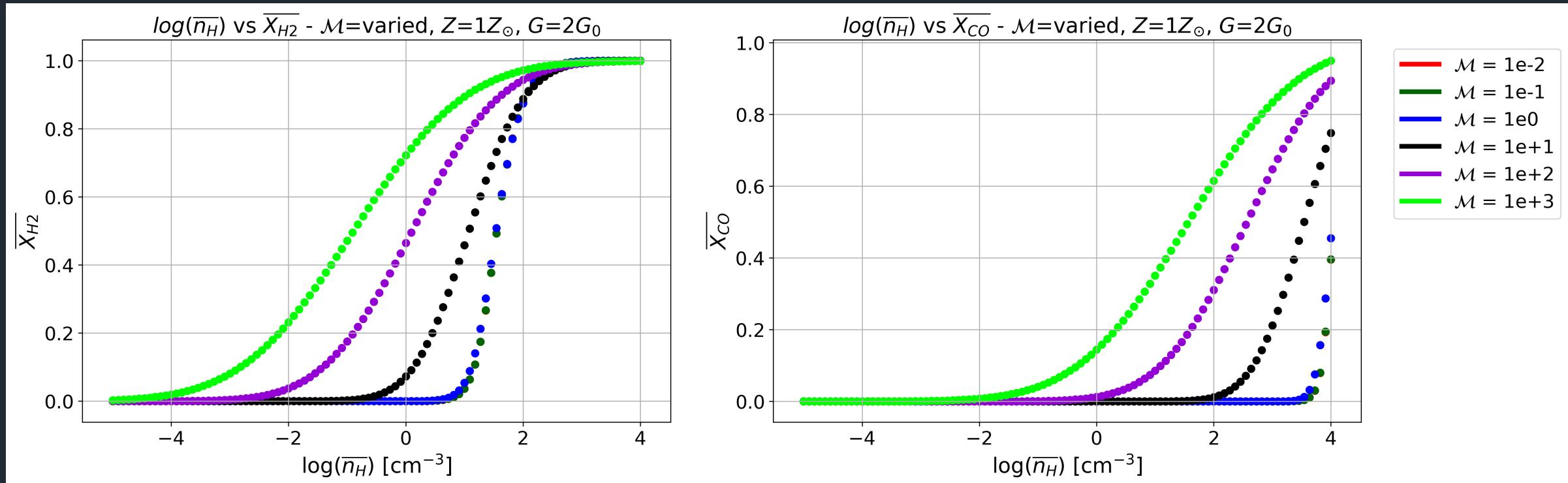
$$M_{H2} = m_p \sum_{cells} (\overline{X}_{H_2} \overline{n}_H) (\Delta x)^3$$

$$\alpha_{CO} = \frac{M_{H2}}{L_{CO}}$$

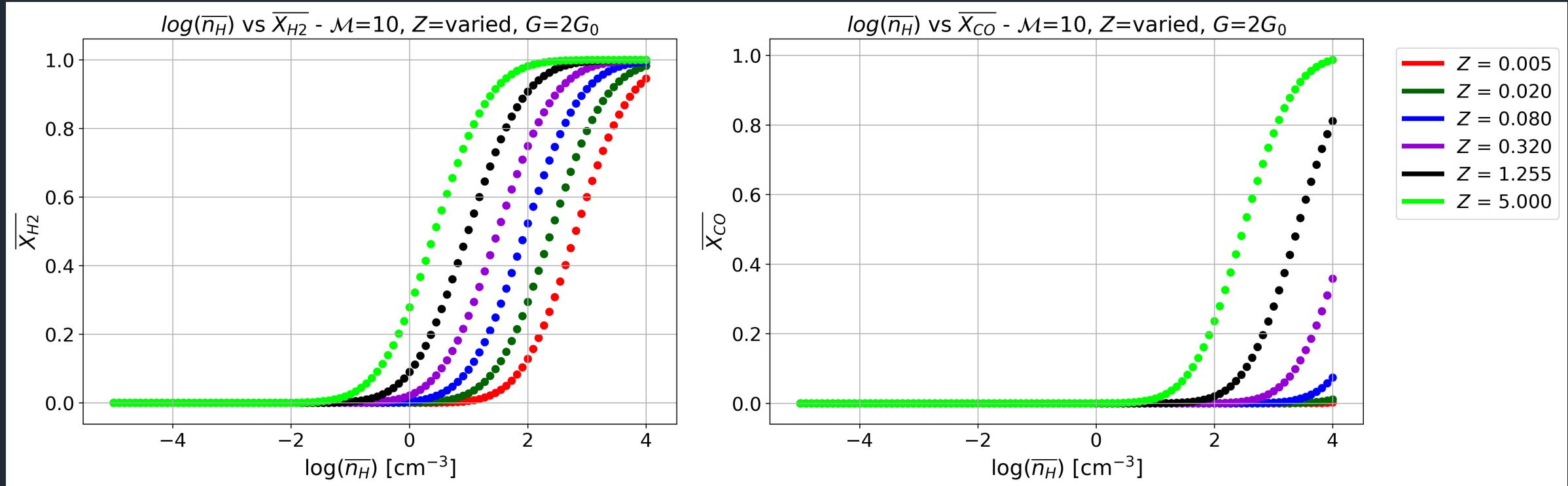
Predictions of the model

- Varying the parameters that control macroscopic properties of the simulation cell $(\mathcal{M}, Z, G_0, \Delta v, \overline{n_H})$ in steps.
- For each such step, the sub-grid model computes $\overline{X_{H_2}}$, $\overline{X_{CO}}$, $\overline{\ell_{CO}}$, it can effectively mimic the grid of values that will be obtained after post-processing the simulation.

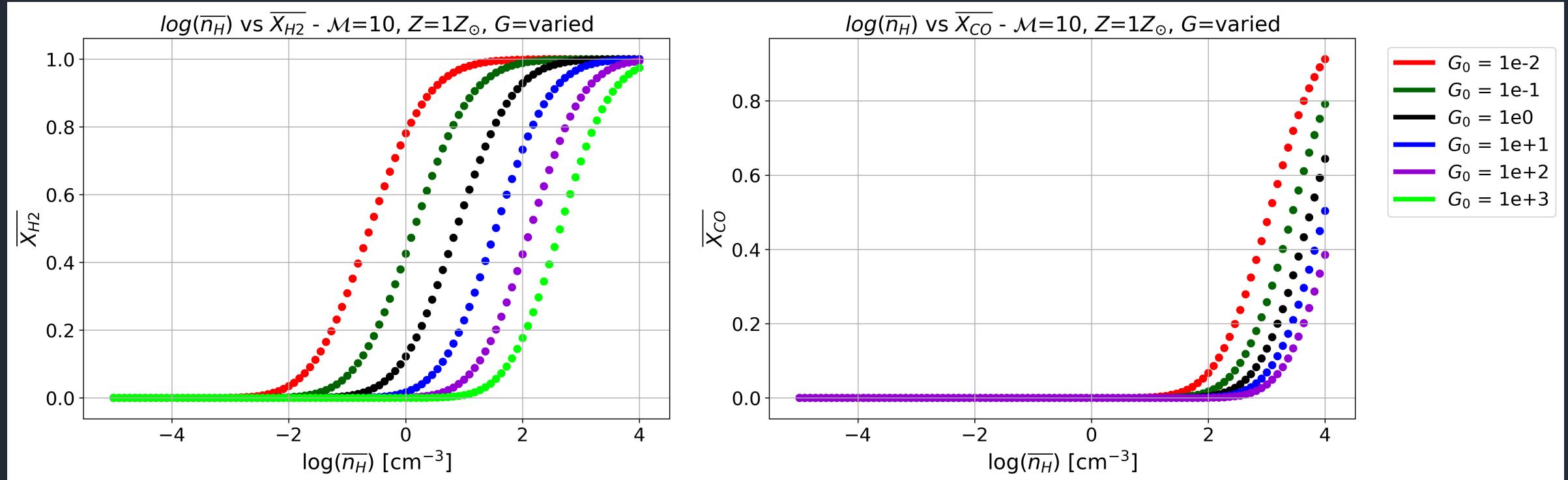
Predictions of the model



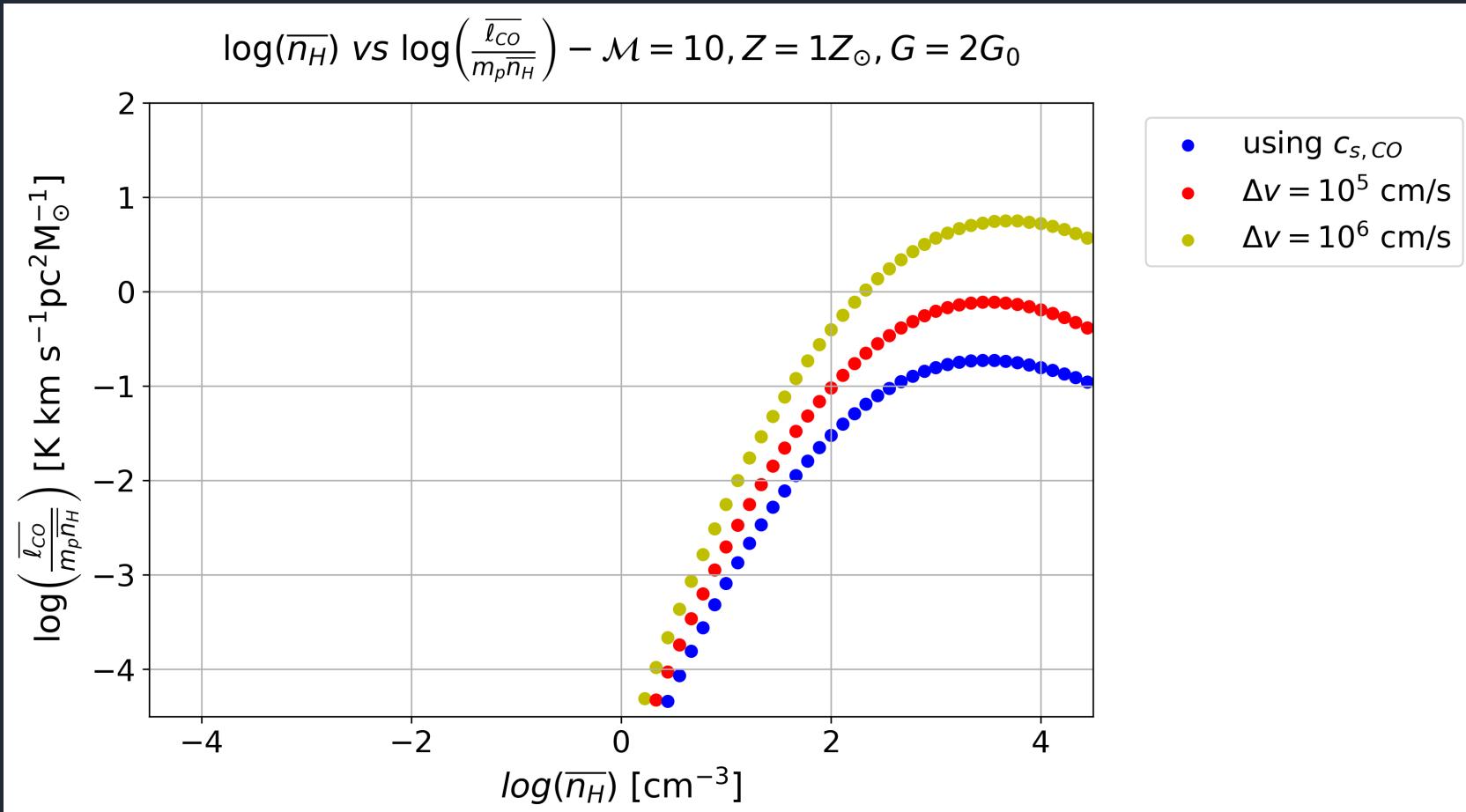
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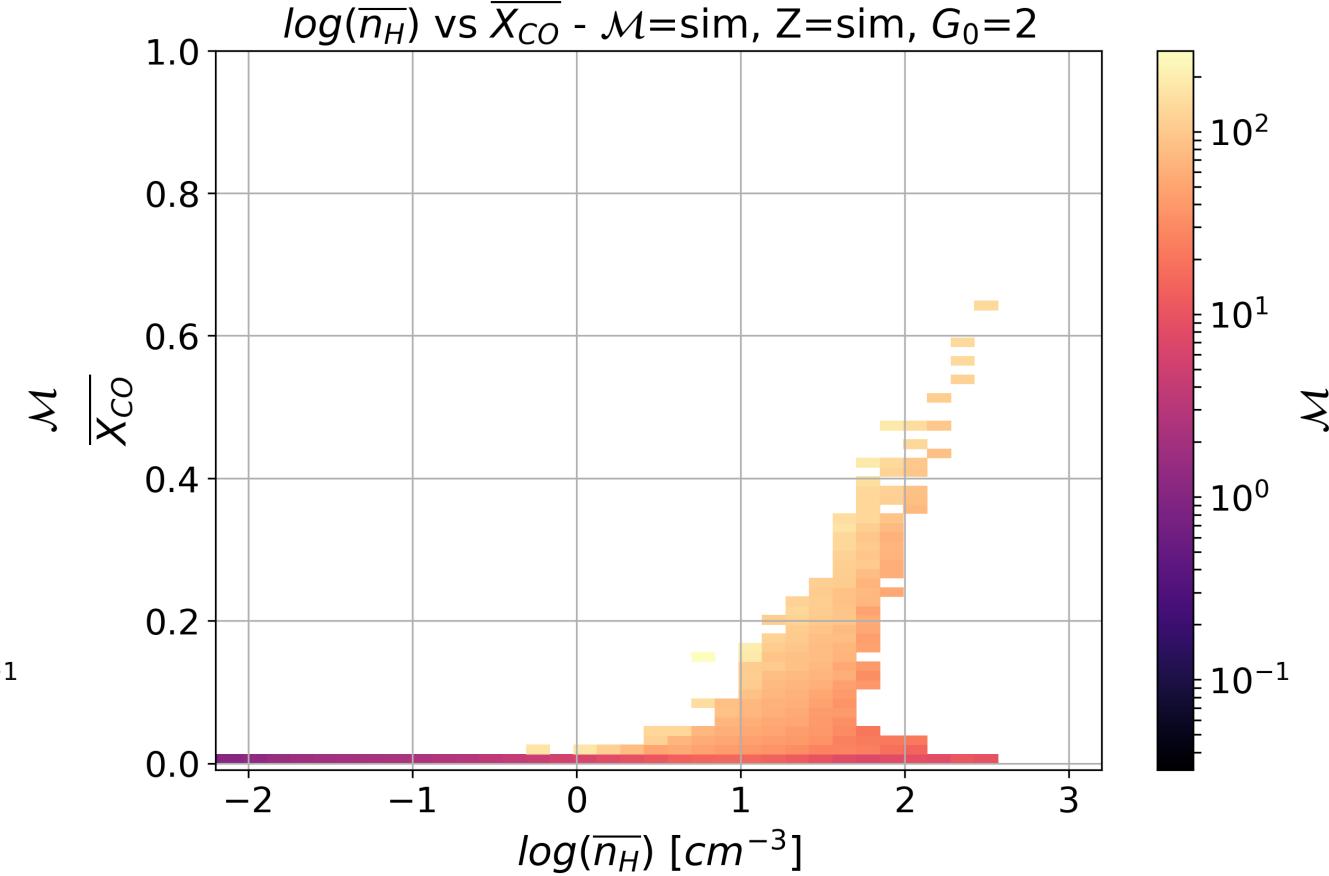
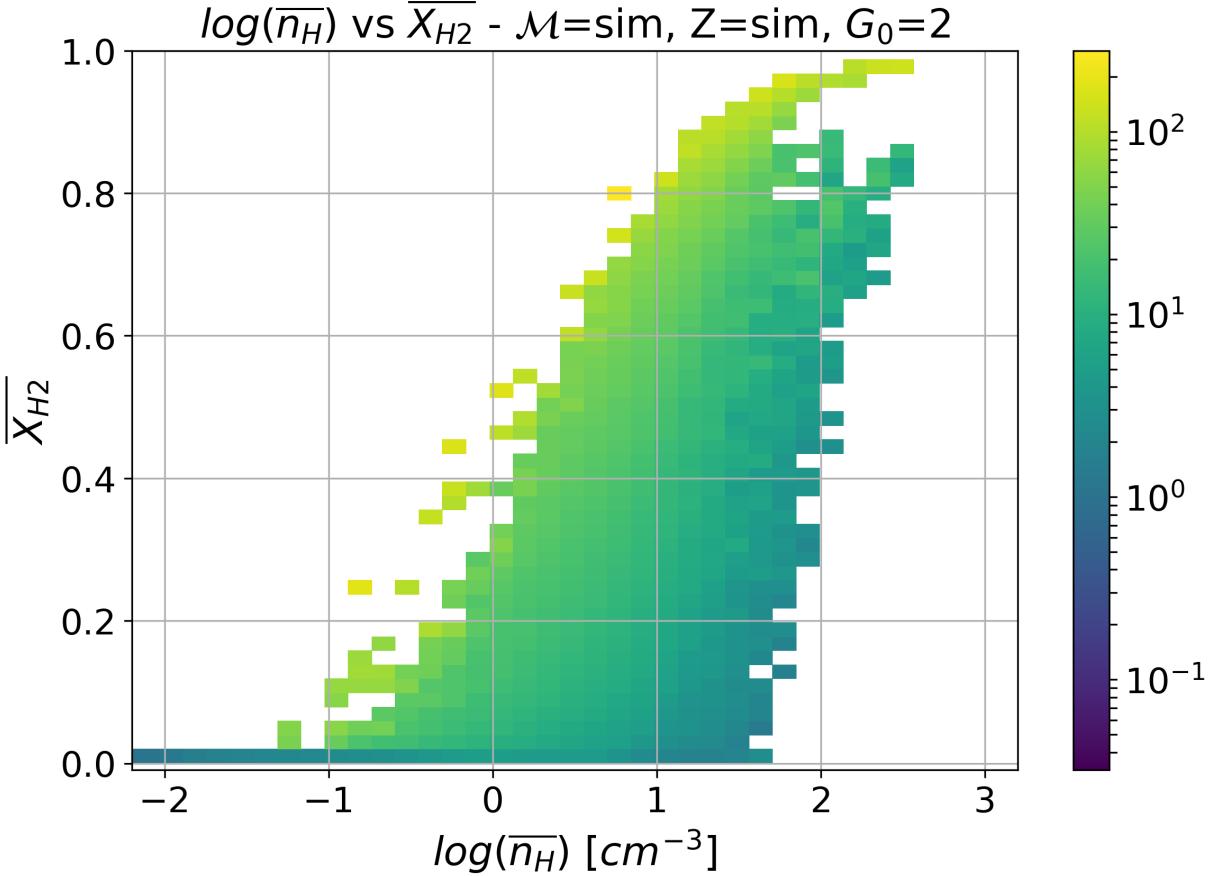
Predictions of the model



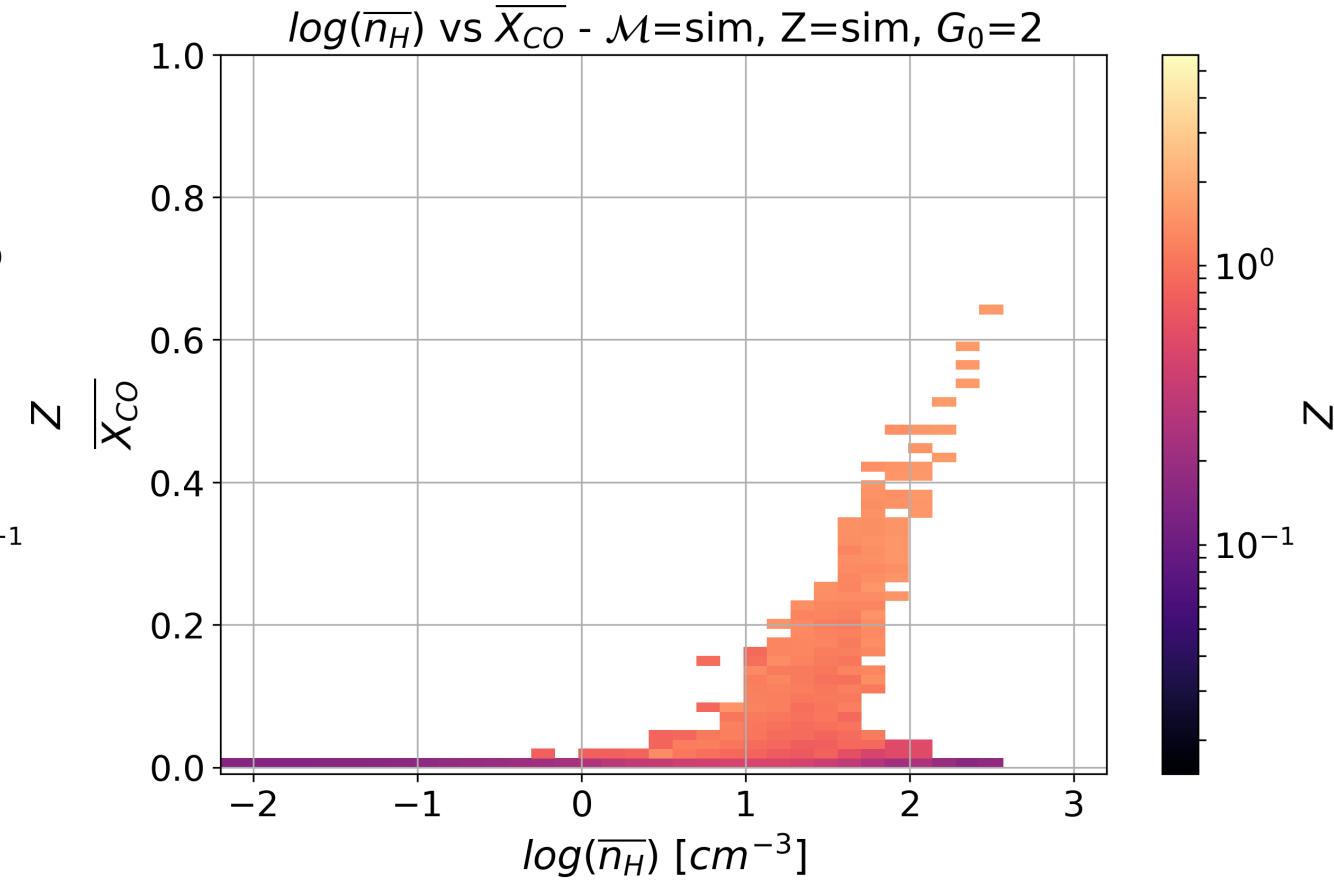
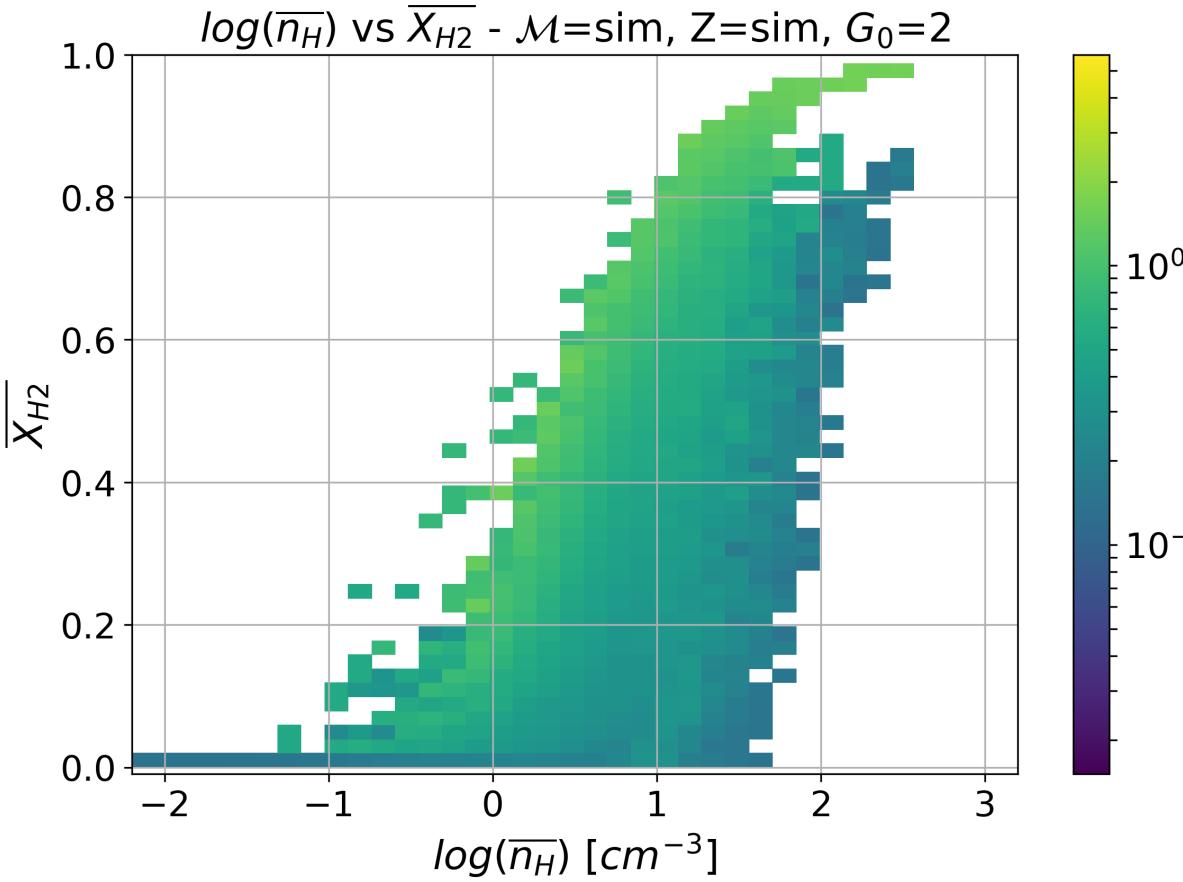
Predictions of the model



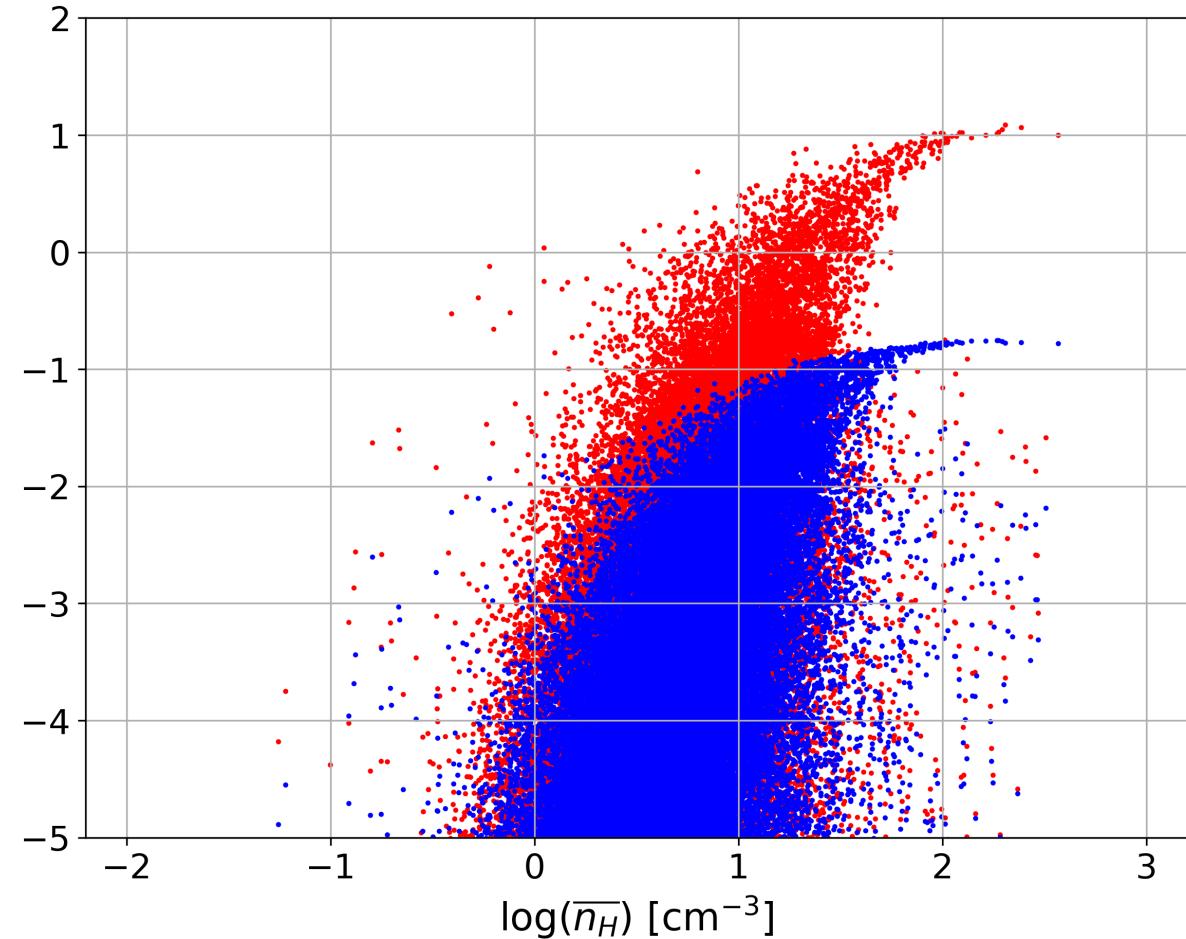
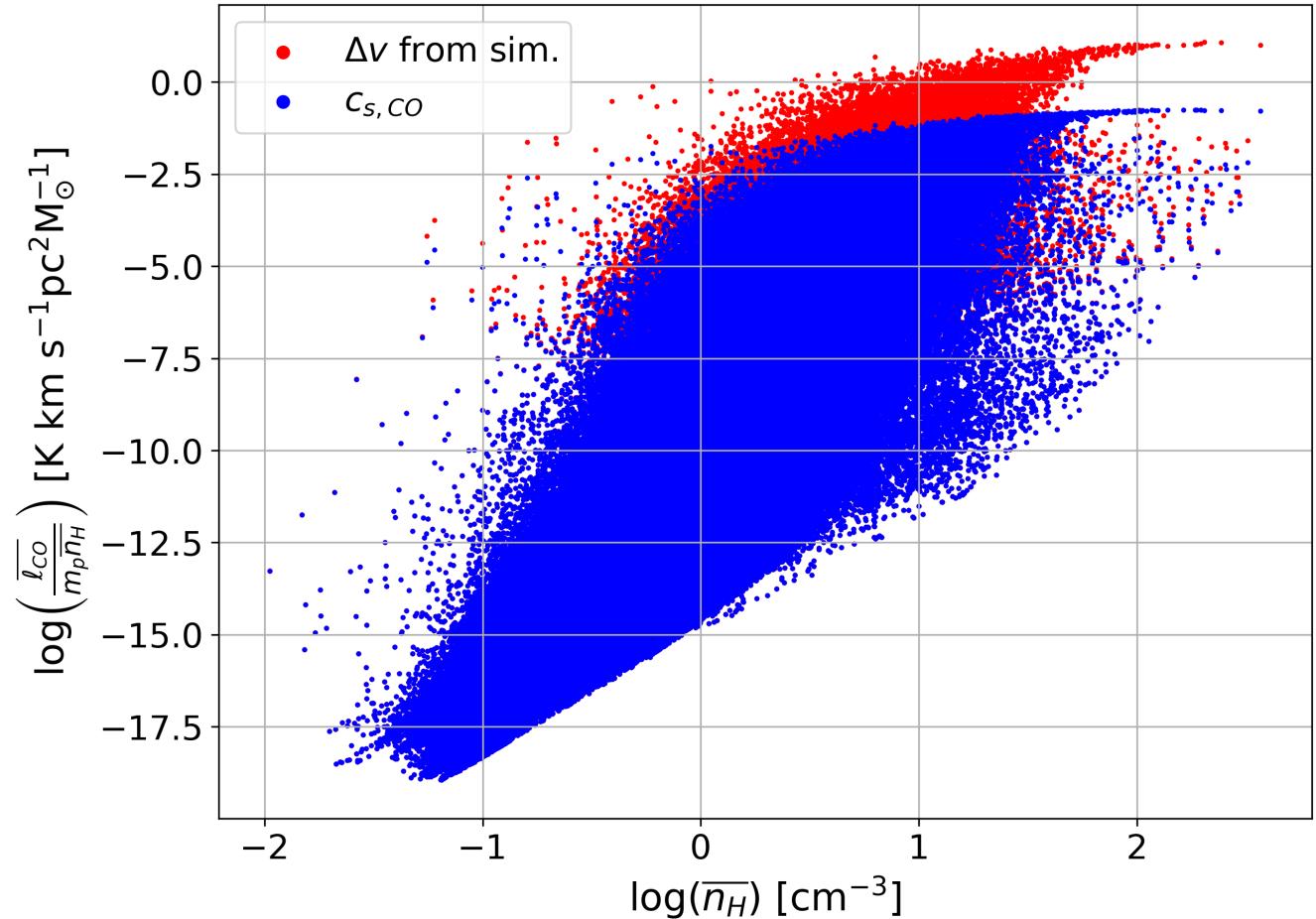
Applying the model on the simulation



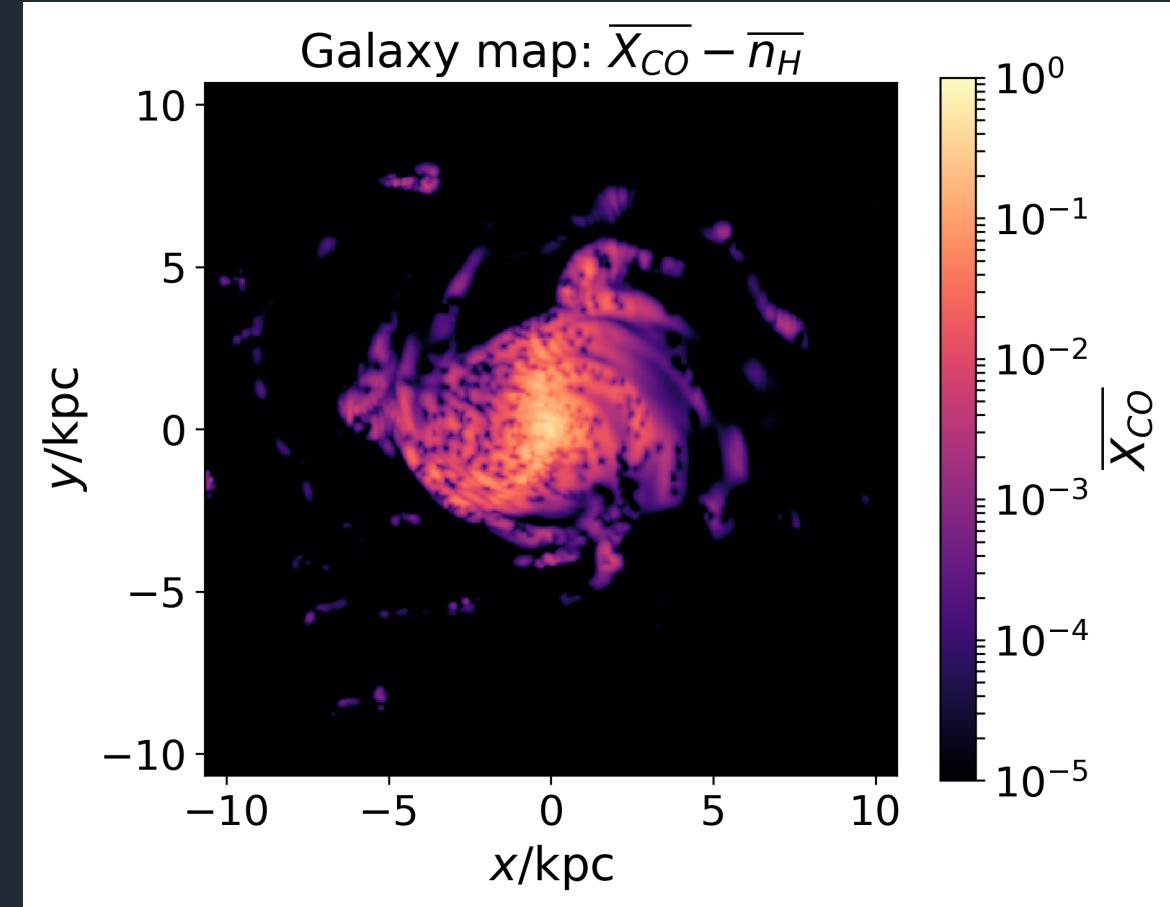
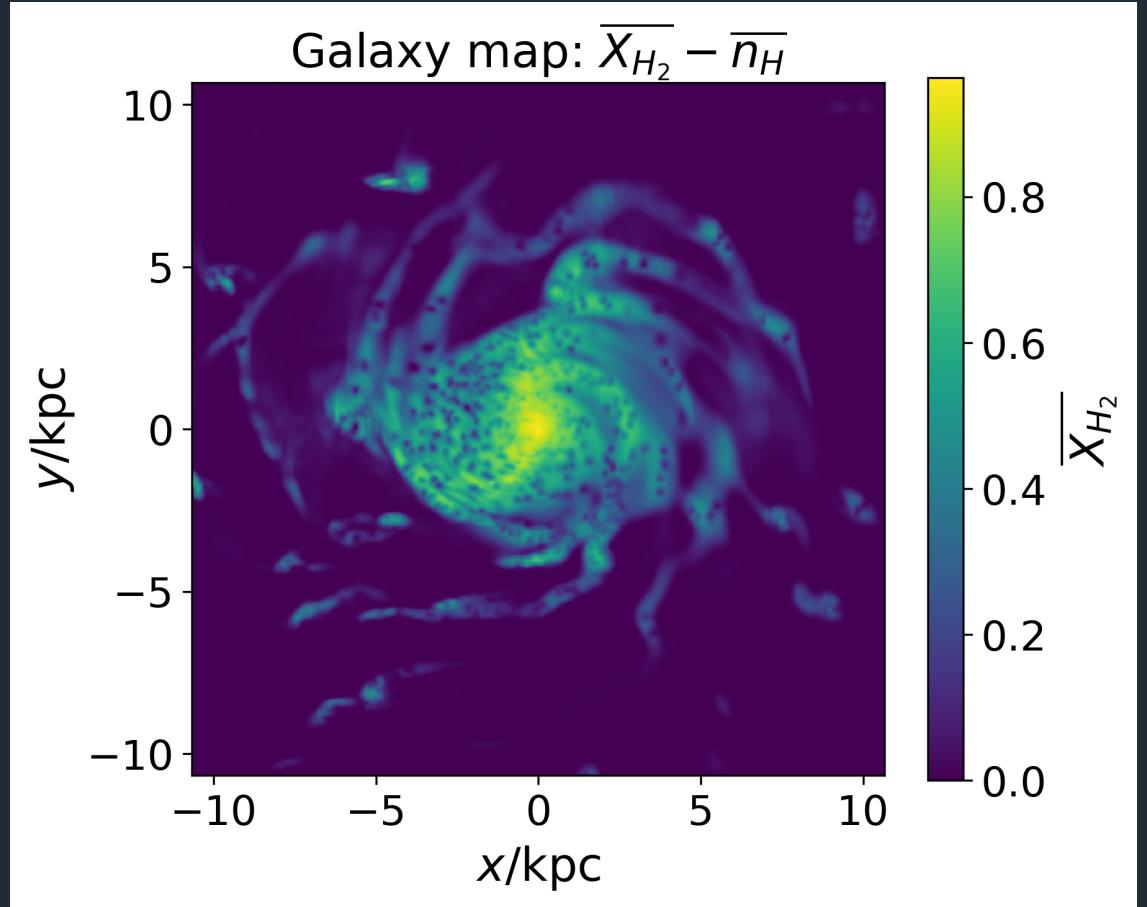
Applying the model on the simulation



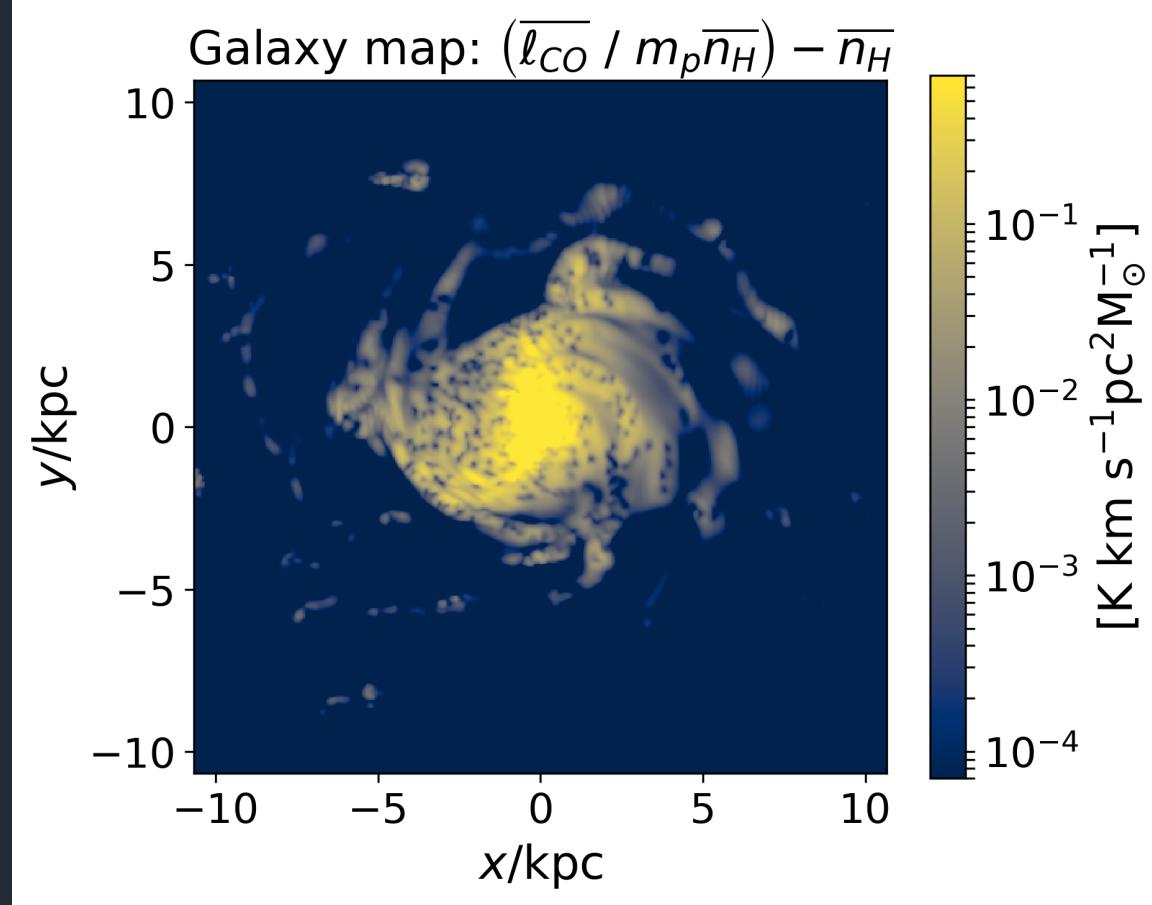
Applying the model on the simulation



Applying the model on the simulation



Applying the model on the simulation



Conclusions

- Self-shielding effect of H_2 - crucial factor
- Large Mach number (\mathcal{M}) and metallicity (Z) - high H_2 and CO formation
- Results using micro-turbulence better than results using thermal motion of the molecules.
- LTE vs non-LTE - not a strong effect for CO(1-0) transition
- In typical Milky Way-like galaxy

$$M_{H_2} \approx 10^9 M_\odot$$

$$L_{CO} \approx 2.5 \times 10^8 \text{Kkms}^{-1}\text{pc}^2$$

$$\alpha_{CO} \approx 4 \text{ M}_\odot(\text{Kkms}^{-1}\text{pc}^2)^{-1}.$$

Conclusions

- $M_{H_2} = 2.9 \times 10^9 M_\odot$
- For thermal microscopic motions of the absorber:
$$L_{CO} = 7.3 \times 10^7 \text{Kkm}\text{s}^{-1}\text{pc}^2$$
$$\alpha_{CO} = 39 M_\odot (\text{Kkm}\text{s}^{-1}\text{pc}^2)^{-1}$$
- For micro-turbulence model:
$$L_{CO} = 1.9 \times 10^9 \text{Kkm}\text{s}^{-1}\text{pc}^2$$
$$\alpha_{CO} = 1.5 M_\odot (\text{Kkm}\text{s}^{-1}\text{pc}^2)^{-1}$$

Conclusions

- For Evolved PDF:

for pure thermal motions: $L_{CO} = 6.1 \times 10^7 \text{Kkms}^{-1}\text{pc}^2$,

$$\alpha_{CO} = 46\text{M}_\odot(\text{Kkms}^{-1}\text{pc}^2)^{-1}$$

for micro-turbulence model: $L_{CO} = 1.1 \times 10^9 \text{Kkms}^{-1}\text{pc}^2$

$$\alpha_{CO} = 2.7\text{M}_\odot(\text{Kkms}^{-1}\text{pc}^2)^{-1}.$$

Further Work

- Assumption - FUV flux in units of G_0 = the SFR of the galaxy simulation in units of $M_{\odot} \text{yr}^{-1}$ - full-scale radiative transfer model needed.
- A sub-grid model for temperature for each sonic length volume element.
- For CN , C^+ HCO , etc., - Higher line transitions, Non-LTE

Power-law PDF due to self-gravity

Defining γ :

$$\gamma = \frac{1 + 2\epsilon \exp(s) - \sqrt{1 + 4\epsilon \exp(s)}}{2\epsilon^2 \exp(s)}$$

$$\epsilon = \frac{t}{t_{ff}(\bar{n}_H)} = 0.4$$

$$s' = \ln \gamma$$

Power-law PDF due to self-gravity

Bin-width in terms of density and time :

$$q = \frac{[1 - \epsilon \exp(s')]^3}{1 + \epsilon \exp(s')}$$

Computing new PDF, & renormalising it to get the final "evolved"-PDF :

$$P'_V(s) = q P_V(s')$$

$$P_V(s) = \frac{P'_V(s)}{\int \exp(s) P'_V(s) ds}$$

Line Transfer - Energy levels & occupation numbers

- For the $CO(1 - 0)$ transition, $E_{10} = E_1 - E_0 = k_B T_{10} = 5.5\text{K}$, which gives $x_1 = 0.4348$ for $T = T_K = 10\text{K}$.
- Note that for $T = T_{\text{CMB}} = 2.73\text{K}$, $x_1 = 0.2767$, suggesting that non-LTE will not be important for this transition.