#### 1 Results from the Sub-Grid Model

### 1.1 Log-normal PDF vs Power-law PDF

Figure-(label) shows the comparison between the log-normal PDF described by equation-?? and the power-law PDF described by equation-??. The density of the cloud is plotted on the X-axis against the PDF on the Y-axis. The log-normal PDF is described by assuming that the cloud is non-gravitating. When self-gravity is included in the formalism, the PDF develops a power-law tail in the high density region of the cloud. This is because as the density grows, the probability of finding denser clumps increases. The evolution of this power-law tail is shown in figure-(label).

## 1.2 Length scale of the absorbing layer

As shown in equation-??,  $\lambda_J \propto \frac{1}{\sqrt{n_H}}$ , i.e., as the density of the cloud increases, the length of the absorbing layer decreases. This is clearly represented in figure-(label).

### 1.3 Molecular fractions of $H_2$ and CO

Self-shielding of  $H_2$  plays an important role in  $H_2$  and CO formation, as discussed in sections-?? and ??. If self-shielding of  $H_2$  is not included in the model, the  $H_2$  formation shifts to a much higher critical density. In fig-(label, nLW vs log nH), the number of photo-dissociating LW photons are plotted as a function of the density of the cloud, for both regimes, without self-shielding of  $H_2$   $(n_{LW})$  and including self-shielding of  $H_2$   $(n_{LW})$ .

In the case without self-shielding, the critical density at which  $H_2$  starts forming, i.e., the density at which the cloud becomes optically thick for the LW photons is at  $n_{crit} \approx 10^4 {\rm cm}^{-3}$ . This is much higher than observed in gas clouds, where  $n_{crit} \approx 10^1 - 10^2 {\rm cm}^{-3}$ . Now if the self-shielding effects are included, as is shown in figure-(label, nLW vs log nH), the critical density cut-off shifts significantly to the lower side of the density scale. In this regime, the critical density  $n_{crit} \approx 10^1 - 10^2 {\rm cm}^{-3}$ , which is in perfect agreement with the observations.

As expected, this shifting of the critical density towards the lower side of the density scale after self-shielding of  $H_2$  is included is mimicked in by the molecular fraction of  $H_2$ . In figure-(label, XH2 and XH2ss vs nH), without self-shielding  $H_2$  starts forming at  $n_{crit} \approx 10^4 {\rm cm}^{-3}$ . But with self-shielding,

 $H_2$  starts forming at  $n_{crit} \approx 10^1 - 10^2 \text{cm}^{-3}$ , which is again what is observed by astronomers. This proves the significance and validity of the self-shielding of  $H_2$ .

Similarly, the molecular fraction of CO is plotted as a function of density. For CO, which typically forms at densities higher than  $H_2$ , the critical density given by the model is  $n_{crit} \approx 10^4 \text{cm}^{-3}$ . This value is in confirmation with astronomical observations. And since the resulting  $n_{crit}$  fro CO is accurate enough, self-shielding of CO is not included in the model.

### 1.4 Line optical depth and luminosity

As discussed in sections-?? and ??, there are to regimes for line broadening - thermal line broadening, and line broadening due to micro-turbulence.

In the regime of thermal line broadening, the isothermal sound speed for CO is used to calculate the line width  $\Delta\nu$ . Whereas in the micro-turbulence line broadening regime, the velocity dispersion  $(\Delta v)$  is used to calculate  $\Delta\nu$ . In figures-(label) and (label), the optical depth and the escape probability for the emitted photons is plotted as a function of the density of the cloud. Three cases are shown - (1) case using isothermal sound speed, (2) case using  $\Delta v$ , where  $\Delta v = 10^5 \text{cm/s}$ , and (3) case using  $\Delta v = 10^6 \text{cm/s}$ .

As seen from the figures, for the case with isothermal sound speed of CO, theoretical depth of the emitted photons is larger than the optical depth in case using velocity dispersion. This translates into the escape probability in figure-(label), where the critical density for the photon to escape is lower than the for the isothermal sound speed case than the cases considering velocity dispersion.

This phenomenon become clearly evident where the line luminosity is plotted as function of density in figure-(label). As expected, the luminosity for the velocity dispersion cases is larger than the isothermal sound speed case.

# 2 Application of the model on a Simulation

#### 2.1 Introduction

The sub-grid model is applied on a cosmological zoom-in hydrodynamical simulation of a galaxy, described in (cite: Michael's paper). The salient features of this simulation are discussed briefly.

The simulation is based on the Adaptive Mesh Refinement (AMR) code RAMSES (cite: Teyssier 2002). AMR is a technique in which the galaxy 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. For example, in the case where the parameter of choice is the density, the denser regions (like the galaxy core) will be divided into much smaller cubical cells, and the less dense regions of the galaxy will be divided into larger cubical cells. This allows to adaptively refine the spatial resolution and lower the computation time.

For each of these simulation cells, the controlling parameters are - Mach number, metallicity, mean gas number density, temperature, turbulent velocity dispersion, and cell size. Each of these parameters are different for each simulation cell. Mach number for each cell in the simulation is calculated as:

$$\mathcal{M} = \frac{\Delta v}{c_s} \tag{1}$$

where  $\Delta v$  is the velocity dispersion of the turbulence in each simulation cell, and  $c_s$  is the isothermal gas sound speed for each simulation cell computed using the temperature of each simulation cell.

The sub-grid model is applied on each of these cubical cells to resolve the microscopic scales in the simulation. For each of the simulation cell, the parameters are sent to the sub-grid model to compute the mean molecular fractions of  $H_2$  and CO, and also the mean line luminosity of CO. For each simulation cell, the mean values are computed as:

$$\overline{X_{H_2}} = \int X_{H_2,ss} \exp(s) P_V(s) ds, \qquad (2)$$

$$\overline{X_{CO}} = \int X_{CO} \exp(s) P_V(s) ds \tag{3}$$

$$\overline{l_{CO}} = \int l_{CO} P_V(s) ds \tag{4}$$

The mean luminosity is then summed over all the simulation cells to

obtain the total luminosity of the galaxy  $L_{CO}$ , such that:

$$L_{CO} = \sum_{cells} \overline{l_{CO}} \tag{5}$$