I

Introduction

Matter between the stars occupies more than 99% of the volume of galaxies and it is referred to as the interstellar medium (ISM); part of the remaining volume is occupied mainly by stars. In addition to these, it is believed that dark matter is a major component of a galaxy, but we will not refer to it in this thesis. Interstellar gas densities range from 10^{-3} cm^{-3} at the outer edge of a galaxy near the intergalactic medium (Bregman 2007), up to 10^{10} cm^{-3} in proto-planetary disks (Mac Low & Klessen 2004).

In terms of mass, the ISM represents about 10% of the total mass of a galaxy, where on average 1% of its mass is in the form of dust. Different densities and thermal conditions can be found in the ISM. The properties of the phases are summarized in Table-1.1. The subject of study in this thesis will be the molecular ISM.

While generally stars are easy to observe since they emit brightly in the visible range of the electromagnetic spectrum, detecting the gas is not as trivial. Molecular or atomic species can be detected by analyzing the emission or absorption spectra. In fact, in order for the emission of the gas to be observed, the emitting species in the gas should be excited so that the various transitions among these internal states can occur; eventually the photons emitted from these transitions are detected by our telescopes. To give a general idea of the sizes of the objects involved, we mention that the typical length scale of a galaxy is on the order of 10 to 100 kpc whereas the sizes of giant molecular clouds, where star formation occurs, range between 0.1 and 100 pc.

phase	density (cm^{-3})	temperature (K)	volume filling factor
Hot ionized medium	$\sim 3 \times 10^{-3}$	$\sim 5 \times 10^5$	0.7
Warm ionized medium	~ 0.3	$\sim 10000 - 8000$	0.2
Warm neutral medium	~ 0.3	~ 8000	0.1
Cold neutral medium	~ 30	~ 50	0.025
Diffuse molecular clouds	$> 100 - 500$	$\gtrsim 25 - 100$	$\sim 10^{-3}$
Dense molecular clouds	$> 10^4$	$\gtrsim 10 - 50$	$< 10^{-3}$

Table 1.1 – Typical gas densities and kinetic temperatures of the phases of the ISM (Tielens 2005, Snow & McCall 2006).

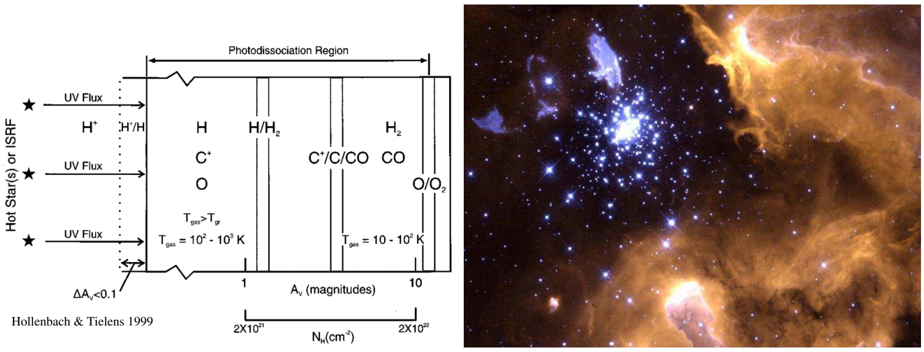
1.1 Chemistry and Radiation

Most of the gas of the ISM is in the form of ionized and neutral hydrogen in the cold and neutral media (labeled with the acronym CNM and WNM, respectively, see Table-1.1. H is the simplest species in the ISM and it is the essential ingredient to form molecular hydrogen H_2. The presence of dust catalyzes the formation of H_2 (Gould & Salpeter 1963). Regions of the interstellar medium where the bulk of hydrogen is in the form of H_2 are known as molecular clouds. The molecular ISM is cold ($\sim$ 10 K) and dense (see Table-1.1), hence the gas is prone to gravitational instabilities which induce the clumpy structure in the molecular ISM; it is believed that stars are born in these unstable regions. The importance of having a good knowledge of the underlying physics and chemistry of star forming regions is key to understanding the overall mechanisms regulating galaxy formation and evolution.

Visible light in molecular clouds is highly obscured by dust, which represents about 1% of the mass of the ISM. Infrared radiation emitted from these clouds which can penetrate large column densities of H_2 ($N(\mathrm{H}) \gtrsim 10^{24}$ cm^{-3}) is used instead of visible light to study star forming regions. H_2 is not useful in probing star forming regions since $T > 300$K is needed to excite its rotational transitions which emit in the mid-IR range.

The far ultra-violet (FUV) radiation (6 eV < E < 13.6 eV) of stars heat the gas surrounding them. Regions of the ISM which are dominated by such radiation are called “photon-dominated regions”. A schematic diagram of a typical PDR, showing the important chemical transitions, is shown in Figure-1.1

In PDRs the surface layer of the clouds is ionized by EUV and heated by FUV photons. The flux of these photons is rapidly attenuated at higher columns of hydrogen ($N(\mathrm{H})$) where the temperatures decrease. As the kinetic temperatures decrease, H^+ recombines with free electrons to form H. At higher column densities H is transformed into H_2 via gas-grain processes. The dust catalyzes the formation of H_2 via a 3-body process, two H atoms and the dust grain. An H atom has a certain probability of sticking on the surface of a dust grain. Once on the surface, it can recombine with another H atom which is also wandering on the surface to form H_2 which then leaves the surface of the grain Gould & Salpeter (1963). In fact, the direct recombination of two hydrogen atoms in gas



Hollenbach & Tielens 1999

Figure 1.1 – *Left*: schematic diagram of a PDR; *right* HST image of the nebula NGC 3603. NASA, Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington), You-Hua Chu (Univ. Illinois Urbana-Champaign)

phase is a very slow process compared to the 3-body processes[1]. In the shielded region of the cloud, where FUV photons have a much lower flux compared to the surface, molecular species other than H_2 form. Many species have been detected (Tielens 2013), we list a few of these that will be discussed in this thesis which are commonly observed in the sub-millimeter and the infrared wavelengths : CO, ^{13}CO, HCN, HNC, HCO^+ , CS, CN, SiO, H_2O, where CO is the most abundant species. The energy levels of these species are excited by collisions with H_2 (para- and ortho-) in addition to H, He, H^+, e^-. It should be noted that excitation due to the collisions with the last two partners are less significant in the shielded region of the PDR because of the low ionization fraction in these environments. The excited populated levels eventually tend to decay to lower states due to spontaneous radiative emission. The necessary densities of the colliding species to sufficiently excite the higher transitions and consequently to enable strong enough emission to be observed depend on their radiative properties. At local thermal equilibrium (LTE) the population densities of the levels between which the transition occurs are determined by the partition function. Usually LTE population densities are achieved whenever the density of the colliding species >> $n_{\rm crit}$, with $n_{\rm crit} \equiv K_{ij}/A_{ij}$, where K_{ij} is the collisional excitation rate coefficient of the transition from the i^{th} to the j^{th} levels and A_{ij} is the spontaneous de-excitation rate, the Einstein A coefficient[2]. Generally, the ISM is not in LTE because $n < n_{\rm crit}$. Thus a good knowledge of the intensities of the emission provides insight on the underlying physical excitation mechanisms of the species (van der Tak 2011).

The main heating mechanism in PDRs is photo-electric heating, which is the heating of the gas due to the photo-electric effect on dust grains. This is the mechanism through which the gas, the FUV radiation and the dust are coupled to each other. Cosmic rays also play an important role in the heating of the gas in the UV shielded region of the

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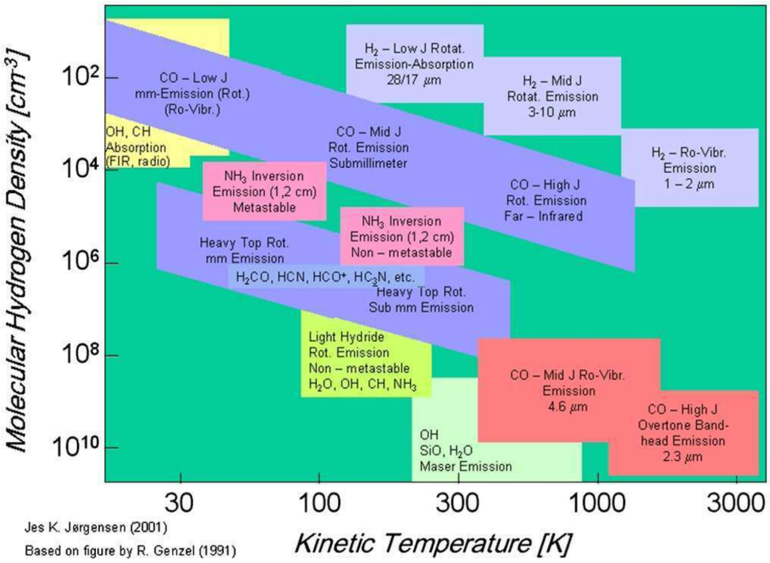
[1] In the chemistry of the early Universe, the only channel for the formation of H_2 are gas phase reactions (Abel et al. 1997, Galli & Palla 1998, Lepp et al. 2002, Coppola et al. 2011)

[2] See Krumholz 2007 for the modified definition of the critical density which takes self-shielding into account



Jes K. Jørgensen (2001)
Based on figure by R. Genzel (1991)

Figure 1.2 – Temperatures and density ranges in the ISM probed by some molecular lines. This diagram is taken from Tielens (2013) which in turn is a modified version from Genzel (1991) and is provided by Jes Jørgensen.

cloud. It has been proposed that the cosmic ray ionization rate in star-burst regions could be as high as 10000 times the ionization rate of the solar neighborhood (Papadopoulos 2010). These regions are referred to as cosmic-ray dominated regions (CRDRs). Moreover, in active galactic nuclei, X-ray heating may play an important role. Similar to cosmic rays, energetic X-rays can penetrate through large columns of hydrogen and H_2 ($N(\mathrm{H}) \gtrsim 10^{24}$) cm^{-3}) and heat up the gas in the regions where UV photons are shielded. These regions are referred to as X-ray dominated regions (XDRs). In addition to these three excitation mechanisms, we will demonstrate in this thesis that mechanical feedback plays an important role in the thermal budget of PDRs which are at chemical and thermal equilibrium. So far we have only mentioned the important heating mechanisms in PDRs. Thermal equilibrium is achieved through fine structure line cooling of atomic and ionized species; the dominant of which is C^+ 158 μm line cooling.

The gas in the ISM can emit at different wavelengths depending on the difference in the energies of the levels involved in the transition. For instance the ionization of a hydrogen atom requires 13.6 eV ($\sim$ 160, 000 K), thus the photons associated with such excitation are in the UV spectrum. On the other hand, transitions of molecular species can be rotational, vibrational and electronic, or various combination of these obeying certain selection rules. Electronic transitions are in general on the order of a few eV. Thus they can be used to probe gas with $T > 10,000$ K. In order to probe low temperature gas $T < 100$ K typical for molecular clouds, transitions with low energies corresponding to such temperatures should be considered. For instance CO has rotational transitions which are commonly observed, with rest frequencies in the sub-millimeter range of the spectrum. In Figure-1.2 the species commonly used to probe different ranges in density and temperature are shown.

1.2 Star formation, Mechanical Feedback and Turbulence

The distribution of stellar masses can empirically be described by a power-law function. This is referred to as the initial mass function (IMF) which determines the probability of finding a star within a certain mass range. Stellar masses range from $\sim$ 0.1 to $\sim$ 100 $M_\odot$where the IMF is a decreasing function of stellar mass. This implies that massive stars are (much) less numerous than low-mass stars. Massive stars are very hot and very bright. Although these stars form about 0.1% the total stellar population, stars with $M \sim$ 100 $M_\odot$ emit about 30000 times ionizing photons compared to stars of lower mass such as the the Sun (Avedisova 1979, Sternberg et al. 2003). The ionizing photons from massive stars, particularly in star forming and star-bursting regions[3], play a very important role in ISM around them where HII regions and PDRs are established.

Another reason why massive stars are important is that they are short lived. They detonate as supernovae liberating typically 10^{51} ergs per event. The shock waves of the blast propagate in its surrounding, disturbing the ISM and inducing turbulence. A few percent of the energy of the supernova is re-absorbed by the ISM which results in heating it up. FUV radiation in PDRs, x-rays in XDRs and cosmic rays in CRDRs heat the ISM locally, where the efficiency of the heating decreases for increasing column densities of H. The main difference in the heating mechanism of these three types of regions of the ISM and regions that are mechanically heated due to e.g. supernovae, is that shocks and turbulence heat the ISM globally on larger scales down to the smallest scales, few pc and up to a kpc. In this thesis, we study the influence of increasing amounts of turbulent heating on the chemical and radiative properties of the ISM in a statistical manner.

1.3 Modelling

Modeling the physical and chemical processes taking place in a galaxy and comparing the results with observations represents a major challenge. While modeling self-gravitating systems is a relatively well defined problem, the hydrodynamic modeling with the various cooling, heating and chemical processes is not. For instance, uncertainties on the reaction rates of some chemical pathways for the formation and destruction of species can affect the solution of the ordinary differential equations that describe the time evolution of the fractional abundances. As a consequence, the cooling and heating mechanisms could be

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[3] Star-bursting regions are regions where the star formation rate is very high > 1 $M_\odot$ yr^{-1}(e.g. Gao & Solomon 2004), compared to the mean estimate of 0.3 $M_\odot$ yr^{-1} in our galaxy (Robitaille & Whitney 2010).

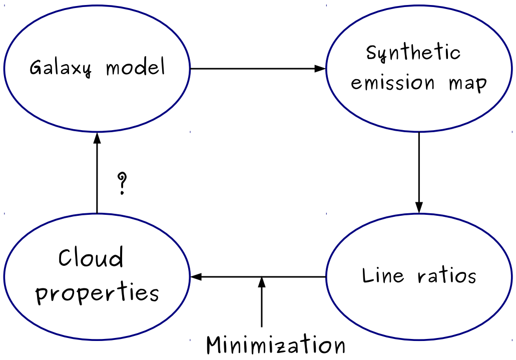

Figure 1.3 – Flow chart diagram of the procedure with which observations are matched to model predictions; The quantity minimized in recovering the “cloud parameters” from the “line ratios” is particular to the approach of this thesis. Any other quantity of interest can be minimized in-order to match the model predictions to the observations.

either under- or over- estimated. Moreover, since $\sim 1\%$ (by mass) of the ISM is composed of dust, all the gas-phase and gas-grains reactions should be taken into account in order to properly describe the chemistry. A high abundance of H_2 in the ISM was suspected for two decades since the early 1940’s. The necessary fast formation rate of H_2 and thus its high abundance in the ISM was explained by Gould & Salpeter (1963), where it was shown that dust catalyzes the reaction of HI on the surface of grains resulting in the expected abundance of H_2 within the dynamical time of a molecular cloud. The high abundance of H_2 was later verified in the 1970’s with the Copernicus satellite.

Another more practical challenge in self-consistent realistic modeling of molecular clouds is the computing times (CPU time) presently required. There have been many attempts of understanding the evolution of molecular clouds, but resolved galaxy-scale self-consistent simulations treating the chemical, radiative transfer and thermal processes accurately and simultaneously require prohibitively long CPU time.

1.4 The Inverse Problem and Diagnostics

Recovering the physical conditions of the gas of the ISM can be thought of as an inverse problem; when given information on the emission, i.e the observed spectra, one can derive the properties of the gas which “might” have caused the observed emission. The general scheme of the modelling procedure is presented in Figure-1.3, where usually by assuming a galaxy model, model (or synthetic) emission are computed and compared to observed line ratios; eventually cloud properties are recovered.

Computing the synthetic maps involves solving a radiative transfer problem, assuming the chemistry is known, or solved for, from the galaxy models. The physics and chemistry incorporated in the modelling provide us with different information, depending on the sophistication of the models and the amount of information and detail with which a galaxy or cloud is to be studied. For instance, using large-velocity-gradient (LVG) models of the line emission (e.g. van der Tak et al. 2007), it is possible to constrain the gas temperature and the density of H_2 and the column density of the species emitting the observed radiation. However, the parameters affecting the underlying physics, such as the FUV flux, can not be constrained using LVG modelling, and the abundances must be assumed in order to derive the mass of the molecular gas. In-order to constrain the UV Flux, PDR modelling is necessary. Observations of luminous and ultra-luminous infra-red galaxies can not be modeled using PDR models alone, since some atomic and molecular line intensity ratios can not be matched using such pure PDRs (e.g. Loenen et al. 2008). Although XDRs models match the emission of LIRGS and ULIRGS in a more satisfactory manner (e.g. Meijerink et al. 2007), in some cases these models are not consistent with the required X-ray fluxes in AGN(for e.g. Maloney et al. 1996, Papadopoulos 2010, Meijerink et al. 2011). In this thesis we use mechanically heated PDR models to attempt matching these line ratios and constrain the amount of mechanical heating needed and find a diagnostic for it.

1.5 Thesis Outline

The work presented in this thesis is divided into two parts. In the first part a parametric study of PDRs is done to probe the effect of mechanical heating under different physical conditions and to identify possible diagnostics for mechanical feedback. In the second part, the PDR models of this parametric study are applied to galaxy models to produce emission maps of molecular species and analyze them. Below, we give an overview of the work done in each chapter.

In **Chapter 2** the effect of mechanical heating on the thermal and chemical properties of PDRs is investigated; in particular, the effect on the kinetic temperature of the gas, abundances, column densities and column density ratios of the molecular species CO, HCN, HNC, HCO^+ and H_2O.

We solve the equilibrium state of all model clouds by using the Leiden PDR-XDR code developed by Meijerink & Spaans (2005). In this code the PDR region irradiated from one side by a UV source is discretized into 1D semi-infinite parallel zones (slabs). The chemical and thermal properties of the zones are solved for iteratively at equilibrium. An escape probability formalism is used to treat the radiative transfer through the discretized slabs. The full internal details of the code are described by Meijerink & Spaans (2005) and the optimization details are discussed in the methods section of Chapter 2. Most possible conditions of the interstellar medium relevant to galaxies are covered by the parameter space of the PDR models. The grids of the models include hydrogen gas density ($1 < n < 10^6\,\mathrm{cm}^{-3}$), FUV radiation field ($0.32 < G_0 < 10^6$) and mechanical heating rate ($10^{-24} < \Gamma_{\mathrm{mech}} < 10^{-16}\,\mathrm{erg\ cm^{-3}\ s^{-1}}$). We find that in steady-state equilibrium clouds mechanical heating plays an important role in determining the kinetic temperature of the gas in molecular clouds. We demonstrate the importance of considering mechanical heating in modelling the ISM of star-burst galaxies and galaxy centers, where the gas temperatures are underestimated by at least a factor of two if mechanical heating is ignored. Since $\Gamma_{\rm mech}$ also affects the abundances of the species, their column densities are varied accordingly. Generally, the column densities of CO, HCN and H_2O increase as a function of $\Gamma_{\rm mech}$. The HNC/HCN integrated column density ratio shows a decrease by a factor of at least two in high-density regions with $n \sim 10^5\,{\rm cm}^{-3}$. On the other hand, the HCN/HCO^+ column density ratio increases by three orders of magnitude. If mechanical heating is not included, predicted column densities of e.g. CO are underestimated, sometimes as in the case of HCN and HCO^+ by a few orders of magnitude. As a lower bound to the influence of $\Gamma_{\rm mech}$, we determined that non-negligible effects are imposed when $\Gamma_{\rm mech}$ is as little as 1% of the UV heating in a PDR.

The chemical and thermal properties of clouds determine the radiation emanating from them. In **Chapter 3** we extend the work done in the previous chapter by investigating the effect of mechanical heating on atomic and molecular lines, and their ratios. We try to use those ratios as a diagnostic to constrain the amount of mechanical heating in a region and also study its significance on estimating the H_2 mass. The emission of the PDR grids are computed assuming the Large Velocity Gradient approximation (Sobolev 1960). The equilibrium state of the PDR models are used as input to RADEX (van der Tak et al. 2007) where the emission is computed in post-processing mode.

We find that line ratios involving CO transitions with $J > 4-3$ are very sensitive to mechanical heating. The emission of these transitions becomes at least one order of magnitude brighter in clouds with $n \sim 10^5$ cm^{-3} and a star formation rate of 1 $M_\odot$ yr^{-1} (corresponding to $\Gamma_{\rm mech} = 2 \times 10^{-19}$ erg cm^{-3} s^{-1}). Rotational transitions of CO with $J < 4-3$ are less sensitive to $\Gamma_{\rm mech}$, but they do become brighter in response to $\Gamma_{\rm mech}$. Generally, for all of the lines we considered, $\Gamma_{\rm mech}$ increases excitation temperatures and causes the optical depth at the line centre to decrease. $\Gamma_{\rm mech}$ affects the emission of high density tracers as well. We find that ratios involving HCN are a good diagnostic for $\Gamma_{\rm mech}$. For instance, the ratios HCN(1-0)/CO(1-0) and HCN(1-0)/HCO^+(1-0) increase to values larger than one whenever $\Gamma_{\rm mech} \gtrsim 5\%$ of the surface heating rate. But in pure PDRs these two ratios are much less than unity. The two major conclusions of this chapter are : (1) line ratios involving low-J to high-J transitions will provide good estimates of the mechanical heating rate, as opposed to line ratios involving only low-J ratios; (2) in determining A_V or equivalently $N_{\rm H}$, the mechanical heating rate should be taken into account. Ignoring $\Gamma_{\rm mech}$ leads to a factor of two to three error in determining A_V, and more than one order of magnitude errors in the estimated density and radiation field.

Emission of CO(1-0) is ubiquitously detected in galaxies and is commonly used to estimate the molecular mass in a galaxy or giant molecular cloud (Bolatto et al. 2013). In **Chapter 4**, we study the effect of mechanical heating on diagnostic line ratios of CO and ^{13}CO in model galaxies. Particularly we determine whether these diagnostic line ratios can be used to probe the presence and constrain the magnitude of mechanical heating in actual galaxies. We make use of the PDR models of Chapter 3 and apply them to the gas of a simulated disk and dwarf galaxy in post-processing mode and produce emission maps for the rotational transitions of the CO molecule and its ^{13}CO isotopologue up to $J = 4-3$. The disk and dwarf galaxies are simulated using solar and $1/5$ solar metallicities. The emission maps of these model galaxies are used to compute line ratio maps of the CO and ^{13}CO transitions. These maps are used to illustrate the effect of mechanical feedback on the physical parameters obtained from the molecular line intensity ratios. One of the conclusions of this chapter is that elevated excitation temperature for CO$(1-0)$ correlate positively with mechanical feedback, which is enhanced towards the central region of both model galaxies. A second important conclusion of this chapter is closely related to conclusion (2) of the previous chapter; namely ignoring mechanical feedback in the heating budget over-estimates the gas density by a factor of 100 and the far-UV flux by factors of $\sim 10-1000$. We find that PDRs that take mechanical feedback into account are able to fit all the line ratios for the central < 2 kpc of the fiducial disk galaxy quite well. In the central region of the disk galaxy, the mean mechanical heating rate, mean gas density, and A_V recovered from these fits agree to less than half dex with their corresponding values in the model galaxy. In applying our technique to the dwarf galaxy, we conclude that single component PDR model fits are not suitable for determining the actual gas parameters of such systems although the quality of the fit line ratios comparable to that of the disk galaxy.

In **Chapter 5** we extend the work of the previous chapter by considering species other than CO and ^{13}CO. We include the rotational transitions with critical densities $n \gtrsim 10^4$ cm^{-3}, particularly $4-3 < J \leq 15-14$ transitions of CO and ^{13}CO, also $J \leq 7-6$ transitions of HCN, HNC and HCO$^+$. In this chapter, we focus only on the disk galaxy, where the density field of the interstellar medium of the model galaxy is re-sampled to account for the emission of gas with densities $> 10^3$ cm^{-3}. The re-sampling is done by assuming the probability density function (PDF) of the density is a log-normal function inferred from the resolved low density scales. We find that in a narrow gas density PDF, with a mean density of ~ 10 cm^{-3}and a dispersion $\sigma = 2.1$ in the log of the density, most of the emission of molecular lines even of gas with critical densities $> 10^4$ cm^{-3}emanate from the 10-1000 cm^{-3}part of the PDF.

Following a similar approach to Chapter 4, we fit the line-ratios of the synthetic emission maps for the central 2 kpc of the galaxy using one PDR model. Since the distribution of the luminosity of the model galaxy, as a function of density, is peaked at gas densities between 10 to 1000 cm^{-3}, we find that one component PDRs fit the various line ratios well. In the second part of this chapter, we investigate the impact of different log-normal density PDFs on the distribution of the luminosity as a function of density. The aim of this exercise it to check the conditions under which significant emission is obtained from gas with densities $n > 10^4$ cm^{-3}, and to test for the possibility of constraining the PDF using line ratios of high density tracers. The Mach number, $\mathcal{M}$, can be related to the dispersion of a log-normal distribution. Hence constraining the density PDF provides a handle on the Mach number which is an important parameter is super-sonically turbulent environments. In our exploration, we find that it is necessary to have a broad dispersion, corresponding to Mach numbers $\gtrsim 30$ in order to obtain significant ($> 10\%$) emission from $n > 10^4$ cm^{-3}gas; such Mach numbers are expected in Luminous Infrared Galaxies (LIRGS) and Ultra Luminous Infrared Galaxies (ULIRGS). By applying our method to grid of line ratios of HCN(1-0), HNC(1-0) and HCO$^+$ (1-0), we show that fitting line ratios of a sample of LIRGS and ULIRGS, using mechanically heated PDRs, we constrain the Mach number of these galaxies to $29 < \mathcal{M} < 77$, which is within the expected range.

In the final chapter we put the work done in the thesis into perspective of recent observations and discuss the importance and possible applications of our models to data obtained by ALMA. We also discuss the major caveats of our present modelling and ways of improving future modelling, the major limitations and some estimates on the requirements for improved modelling of the chemistry and the radiative transfer.