Diagnostics for mechanical heating in star-forming galaxies

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Title: Diagnostics for mechanical heating in star-forming galaxies
Issue Date: 2015-06-03

VI

General Discussion and Prospects

6.1 Thesis summary

In this thesis, I studied the effects of mechanical heating ($\Gamma_{\rm mech}$) due to dissipating shocks and turbulence on diagnostics of regular star-burst galaxies (L_{IR} (8-1000 μm) ~ 10^{9-10} $L_\odot$) as well as their extreme counterparts that are classified as luminous infrared galaxies (LIRGs) (L_{IR} (8-1000 μm) ~ 10^{11} $L_\odot$) and ultra-luminous infra-red galaxies (ULIRGs) (L_{IR} ~ 10^{12} $L_\odot$). These galaxies exhibit much higher star formation rates, up to 1000 $M_\odot$ yr^{-1}, compared to 0.01 $M_\odot$ yr^{-1}in a quiescent spiral galaxy such as the Milky way. The main questions I addressed in this thesis are: a) To what extent is mechanical heating important for the thermal and chemical balance of the ISM in star-burst galaxies? b) Does the inclusion of mechanical heating significantly change the interpretation of commonly used diagnostics such as line emission intensity ratios among [CI], [CII], ^{13}CO , CO and other high-density tracers? In particular, how important is mechanical heating in constraining cloud parameters in star-burst galaxies? c) How well can molecular line emission be used to probe the density distribution of super-sonically turbulent clouds in star-burst regions caused by shocks of supernova explosions and stellar outflows ?

In the scientific literature several authors have produced tables and diagrams of atomic and molecular line emission which enable the user to constrain the physical properties of PDRs, mainly the gas density and the FUV flux (e.g, Kaufman et al. 1999, Meijerink et al. 2007). These PDR models are partly able to explain multitransition CO observations of star-forming regions in galaxy centers (for e.g. Israel & Baas 2002), where the main problem arises in modeling the bright emission of CI which is consistently brighter in observations (Israel & Baas 2002). But as more data became available for LIRGS and ULIRGS by the Herschel Space Observatory (Pilbratt et al. 2010), it was clear that additional physical and (or) chemical processes must be included in these models to explain observations of modest star-busts in galactic nuclei (e.g. Israel & Baas 2003) as well as extreme star-forming regions (e.g. Loenen et al. 2008). For instance PDR models are unable to clearly define the parameters of the gas components of the star-bursts in galaxy centers using relative line intensities of ^{13}CO with [CI] and [CII] (for e.g. Israel & Baas

2002). The urge of using more sophisticated PDR modeling involving additional heating sources became evident in the work done by Loenen et al. (2008) and more importantly with the new *Herschel* data for high-J rotational lines of CO and other relevant molecular species (Israel & Baas 2002, Pilbratt et al. 2010, González-Alfonso et al. 2010, van der Werf et al. 2010, Meijerink et al. 2013).

In answering the questions we posed above, we extended the works by Meijerink et al. (2007), Loenen et al. (2008) and Meijerink et al. (2011) by including mechanical feedback as a free parameter in the heating budget of the PDR models. We constructed grids that allowed for constraining cloud parameters over the same parameter space considered by Kaufman et al. (1999), where pure PDR models without any mechanical heating were used to study the star-forming regions of M82, NGC 278, and the Large Magellanic Cloud.

In **Chapter-2** we explored a wide range of parameter space covering densities ranging from 1 to 10^6 cm^{-3} and FUV fluxes ranging from 1 G_0, for e.g. in the solar neighborhood, to fluxes of 10^6 G_0 typical at distances of 0.1 pc from an O star that are common in star-bursts. We concluded that mechanical heating for regions where star-formation rates ranging from SFR $\sim$ 0 to $\sim$ 1000 M$_\odot$ yr^{-1} corresponding to $10^{-24} < \Gamma_{\rm mech} < 10^{-16}$ erg cm^{-3} s^{-1} impacts the thermal and chemical balance strongly. For example, an order of magnitude increase in the kinetic temperature of steady-state equilibrium clouds is not uncommon in the molecular zone. Moreover, in regions with star formation rates as large as $\sim$ 1000 M$_\odot$ yr^{-1}, the H/H_2 transition does not occur. As a consequence the abundances of other molecular species whose formation relies on the abundance of H_2 are also affected in these photo-dominated regions, leading to a strong reduction in their column densities. Thus, to answer question (a), we found that mechanical heating strongly affects the equilibrium state of clouds. As a lower bound to the influence of $\Gamma_{\rm mech}$, we determined that for $\Gamma_{\rm mech} \sim 0.01\ \Gamma_{\rm photo}$ the chemistry of the PDRs is significantly changed.

The emission of species depends primarily on their abundance and on the physical properties of the clouds, such as the kinetic temperature. In **Chapter-2** we found that $\Gamma_{\rm mech}$ also affects the abundances of chemical species and their column densities. We also found that 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 $n \sim 10^5$ cm^{-3}. On the other hand, the HCN/HCO^+ column density ratio increases by three orders of magnitude. We built on these results in **Chapter-3** where we calculated the emission grids of the atomic fine-structure lines of [OI], [CII], and [CI] in addition to the various molecular line transitions of CO, ^{13}CO, HCN, HNC, HCO^+, CN, and CS.

So far this has been a forward problem, where the effect of mechanical heating was probed on the physical and chemical properties of clouds. Typically, these properties are inferred from molecular line emission of star-forming regions where the measurements are matched against the product of models of such regions. We found 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 $\Gamma_{\rm mech}$ = 2×10^{-19} erg cm^{-3} s^{-1}). The emission of the transitions of the species emanating from the

PDRs were computed using Large Velocity Gradient (LVG) models (e.g. Sobolev 1960, Henkel et al. 1983, Jansen et al. 1994, Hogerheijde & van der Tak 2000, van der Tak et al. 2007, Krumholz 2014). The input needed by these LVG models, for e.g. the column density of the species and the kinetic temperature of the gas, were extracted from the PDR models as averaged quantities, where the main assumption was that the line width is constant and is not related to the mechanical heating rate. Rotational transitions of CO with $J < 4-3$ are less sensitive to $\Gamma_{\rm mech}$compared to the $J > 4-3$ transitions, however 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 center to decrease; this effect is due to the reduced level populations for the lower excited states at higher temperatures. $\Gamma_{\rm mech}$ affects the emission of high density tracers as well. We found 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 photo-electric heating rate, while in pure PDRs these two ratios are much less than unity. The two major conclusions of chapter-3 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.

En-route to answering (c), we applied mechanically heated PDR models to the substructure of the gas of simulated galaxies in Chapters 4 and 5. Two fiducial model galaxies were examined: a small disk galaxy of solar metallicity and a lighter dwarf galaxy with 0.2 $Z_\odot$metallicity. Emission maps of CO and ^{13}CO (up to $J = 4-3$) were constructed for both galaxies in Chapter-4. This work was extended in Chapter-5 where emission maps up to $J = 15-14$ were constructed, in addition to emission maps of the high density molecular tracers HCN, HNC and HCO^+up to $J = 7-6$. These maps were used to investigate the occurrence and the effects of mechanical feedback on recovering the physical parameters obtained from molecular line intensity ratios. The general conclusion of both chapters was that molecular line emission are very useful in constraining mechanical heating, especially in the central regions of galaxies. Moreover, since high-J to low-J line ratios are very sensitive to mechanical heating, they are good diagnostics for it. Possible degeneracies with XDR models will be discussed in the Section-6.4.

One of the important conclusions of Chapter-4 is that elevated excitation temperature for CO$(1-0)$ is correlated positively with mechanical feedback, which is enhanced towards the central region of the model galaxies. A second important conclusion of this chapter is closely related to the conclusion of Chapter-3; namely ignoring mechanical feedback in the heating budget over-estimates the derived gas density by a factor of 100 and the derived far-UV flux by factors of $\sim 10-1000$. We found that PDRs that take mechanical feedback into account are able to fit all the line ratios of CO and ^{13}CO quite well, up to the transition $J = 4-3$, for the central < 2 kpc of the fiducial disk galaxy. In the central region of the disk galaxy, the mean mechanical heating rate, mean gas density, and A_V recovered from these line ratios to less than half dex with their corresponding values in the model galaxy. In applying our modeling technique to the typical dwarf galaxy, we concluded 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 recovering the cloud parameters in Chapter-4 it was assumed that the gas has uniform properties, or is composed of a small number of uniform components. In reality, on the scale of a galaxy or on the kpc scale of star-bursting regions common in LIRGS and ULIRGS, the gas density follows a continuous distribution. The exact functional form of this distribution is currently under debate, but it is believed that in star-burst regions, where the gas is thought to be super-sonically turbulent due to e.g. outflows and shocks, the density distribution of the gas is a log-normal function. It is also possible to have a more relaxed power-law distribution in models of supersonic turbulence where the effective equation of state has a polytropic index, γ, less than one (e.g. Nordlund & Padoan 1999). In **Chapter-5** we demonstrated that generalizing our models to fit line ratios by considering a set of clouds following an log-normal density distribution, it is possible to constrain the type of the turbulence in star-bursting galaxies. Particularly we demonstrated that the emission of high density tracers can be used to constrain the density distribution of super-sonically turbulent regions and the mach number as well which is tightly coupled to the width of the density distribution. We found that in a narrow gas density PDF, with a mean density of $\sim$ 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. 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 found that one component PDRs fit the various line ratios well. In our exploration, we found 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 LIRGS and ULIRGS. By applying our method to grid of line ratios of HCN(1-0), HNC(1-0) and HCO^+(1-0), we showed that it is possible to fit line ratios of a sample of LIRGS and ULIRGS using mechanically heated PDRs. We constrained the Mach number of these galaxies to be between $29 < \mathcal{M} < 77$, which is within the expected range.

In the following two sections we present two case studies where the grids of Chapters-2 and 3 have been applied to recent observation of NGC 253 and Arp 299. For these systems it has been shown by Rosenberg et al. (2014a,b) that mechanical heating is necessary for fitting and interpreting observations in such violent star-forming regions.

6.2 Application to NGC 253

NGC 253 is among the brightest galaxies that have been studied in wavelengths ranging from radio waves to X- and gamma rays. It is also one of the classic galaxies, similar to M82, Mrk 231 and Arp 299, that has very strong emission in the far-IR and sub-mm wavelengths due to the strong star-burst activity in the large molecular clouds that are present in its central kilo-parsec nuclear region (Israel et al. 1995, Mauersberger et al. 1996, Houghton et al. 1997, Bradford et al. 2003, Martín et al. 2009). Rosenberg et al.

(2014a) applied the models developed in Chapters 2 and 3 to recent observations of the ^{12}CO ladder (up to J=13-12) and the ^{13}CO (up to J=6-5) by Herschel, accompanied by older ground based observations of HCN and HNC by the James Clerk Maxwell Telescope (JCMT). They showed that mechanically heated PDR models successfully fit these observations where other models, such as pure PDR models, perform poorly.

Some of the key physical parameters of the gas derived from the observations of ^{12}CO and ^{13}CO in the central region of NGC 253, indicate a kinetic temperature of 120 K and an H_2 density of 4.5×10^4 cm^{-3} (Bradford et al. 2003). These estimates are reinforced by other observations of HCO^+ and HCN which predict a similar range in the density and temperature (Paglione et al. 1995, 1997). The two main suggestions for such high excitation temperatures, for otherwise cold $\sim$ 10 K molecular clouds, are heating by cosmic rays (Bradford et al. 2003) and heating by large-scale low-velocity shocks (Martín et al. 2006).

Rosenberg et al. (2014a) attempt to fit the full set of observations by Herschel and JCMT using : a) three-component LVG models only b) three component pure PDR models c) various combinations of composite PDR, mechanically heated cosmic ray dominated PDR (mCDR) and mechanically heated PDR (mPDR) models. In the case of LVG modeling only, the derived CO column density and the total gas mass were quite uncertain. This is mainly attributed to the fact that the fitting problem is over-determined, i.e., degenerate due to the large number of free parameters in the LVG modeling compared to the available observations (see Section 4.1 by Rosenberg et al. (2014a)). In the case of multi-component PDR modeling the derived mass of the clouds was about 30 times higher than previous estimates. Since the column density of H_2 is proportional to the gas mass, the over estimation of the gas mass was attributed to the high visual extinctions needed to match the bright emission of the High-J transitions due to the "un-accounted for" excitation source. Moreover, the fits of the high density tracers of HCN and HNC were poorly matched using these PDR only models. This led to the third attempt of considering mCDR and mPDR models, where the models proposed in this thesis have been used (see Figure-6.1).

The central region of NGC 253 is a fast star-forming region, i.e. a star-burst, where massive stars are common. These stars are short lived and end up detonating as supernovae, that are sources for cosmic rays. Supernovae cause wide spread shocks and turbulence, hence in modeling such environments it is natural to consider not only CRDRs as proposed by Papadopoulos et al. (2011), but also mCDRs as suggested by Meijerink et al. (2011). Since NGC 253 does not harbor an X-ray bright AGN (Pietsch et al. 2000), X-ray heating was not considered in the analysis by Rosenberg et al. (2014a). Bradford et al. (2003) has proposed that cosmic rays are responsible for most of the molecular gas excitation in NGC 253. Thus, Rosenberg et al. (2014a) used various combinations of mCRDs and mPDRs to model these new observations by Herschel. Among these combinations the best fitting model corresponds to the one in which two mPDR and one PDR models have been included, as shown in the right panels of Figure 6.2.

This model fits all the ^{12}CO, and ^{13}CO transitions within the error bars. In addition, the fluxes of the HCN and HNC transitions are much better fit compared to the two other cases, where these fluxes are over-estimated by at least a factor of two. By comparing all

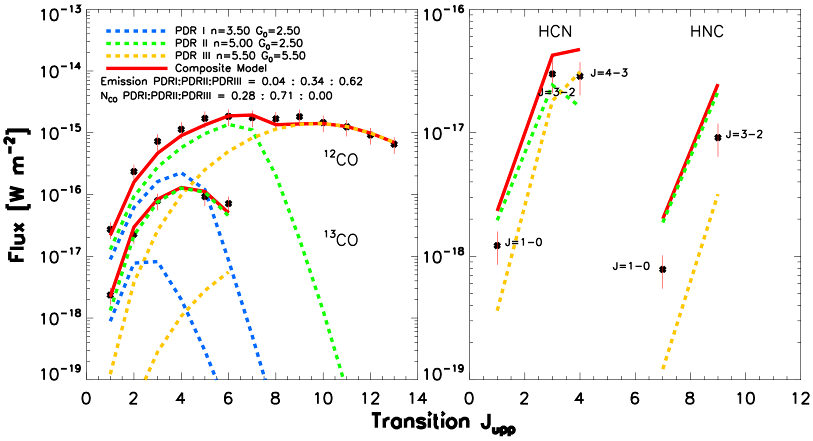

Figure 6.1 – Left: ^{12}CO and ^{13}CO excitation ladders, right: HCN and HNC excitation ladders of NGC 253 with flux of each transition plotted as black asterisks with red error bars. In blue, green and yellow dotted lines we plot the PDR I, II and III ISM phases with their filling factors. The composite model is plotted with a red solid line. The model density, G_0 and column density are shown in the legend along with the relative contribution of each phase in terms of emission and column density.

three panels, it is evident that mechanical heating is necessary to reproduce the observed emission, regardless of the amount of cosmic rays used in the modeling. This finding is similar to that of Nikola et al. (2011) in NGC 891 and Hailey-Dunsheath et al. (2008) for NGC 253 itself, where the emission of mid-J CO transitions have been modeled using a combination of micro-turbulence, shocks and PDRs.

6.3 Application to Arp 299

The mechanically heated PDR models developed and presented in this thesis have also been used by Rosenberg et al. (2014b) to explain the observational data collected by *Herschel* on Arp 299.

Unlike NGC 253, Arp 299 is a system of two colliding galaxies hosting three active galactic nuclei undergoing intense star formation. For this system several observations are available both by *Herschel* (PACS and SPIRE spectrometers) and JCMT. The former provided information about high-J CO lines (up to $J = 20-19$) (Rosenberg et al. 2014b), while for the latter ^{13}CO and HCN lines have been observed. The main difference between these observations and those of NGC 253 is the higher number of ^{12}CO transitions available. This is also true for HCN, where in this case HCN $J = 4-3$ has been detected. Several models were applied by (Rosenberg et al. 2014b) to explain the observed lines detected by *Herschel*; in particular, many heating mechanisms have been introduced to explain the excitation of the high-J transitions. Heating due to cosmic rays, X-rays and

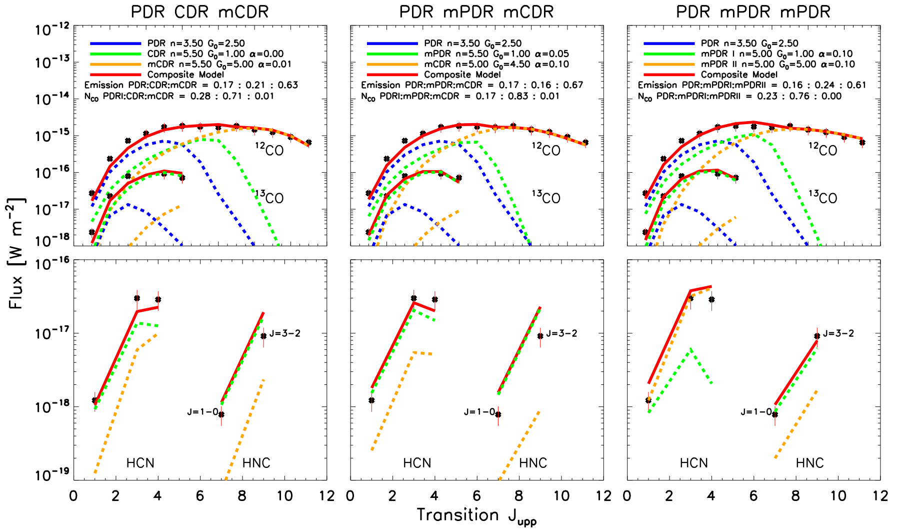

Figure 6.2 – ^{12}CO and ^{13}CO (top) with HCN and HNC (bottom) excitation ladders of NGC 253 with the flux of each transition are plotted as black asterisks with red error bars. In blue, green and yellow dotted lines PDR/CDR/mCDR (left), PDR/mPDR/mCDR (center), and PDR/mPDR/mPDR(right) ISM phases with their filling factors are plotted. The composite model is plotted with a red solid line. The model H_2 density [log cm^{-3}], G_0 [log Habing flux], and percentage mechanical heating (α) are shown in the legend along with the relative contribution of each phase in terms of emission and column density.

mechanical heating were considered.

In particular, mechanically heated Cosmic Rays Dominated Regions (mCDR) models overestimate the observed line intensities; the same results can be obtained for the HCN lines in X-rays dominated regions (XDR) models where the discrepancy reaches more than one order of magnitude (see Fig. 6.3). In a similar approach to the case of NGC 253 presented in the previous sub-section, mPDR models fit the observed ladder for high-*J* transitions within the error bars both for CO, ^{13}CO and HCN. This indicates the importance of mechanical heating in interpreting observations of violent star-bursting galaxies, especially for high-*J* transitions.

6.4 Prospects

6.4.1 Other possible applications

NGC 253 and Arp 299 are two galaxies which have been heavily studied due to their appealing property of being extremely bright in almost all parts of the electromagnetic spectrum. This makes them an ideal laboratory for astronomers to study star forming regions. Those galaxies have been recently observed by Herschel as many other star-

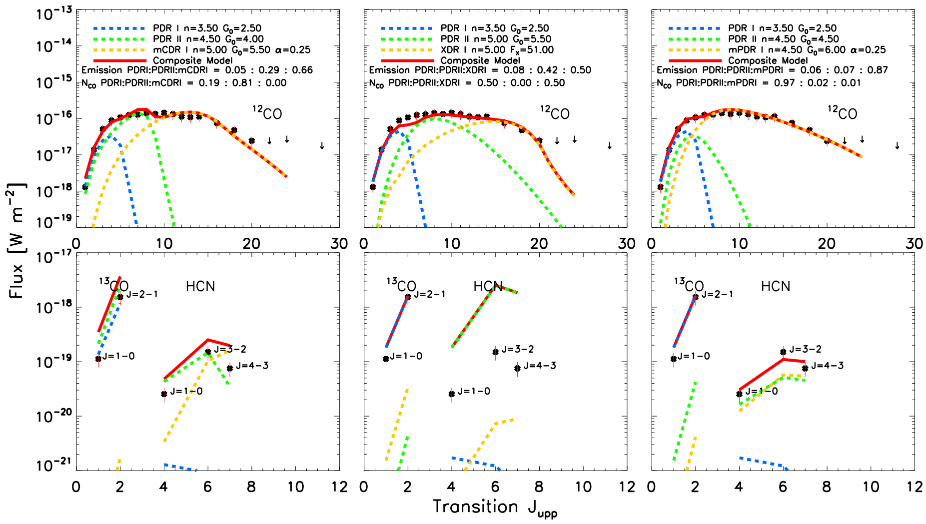

Figure 6.3 – ^{12}CO (top), ^{13}CO, and HCN (bottom) excitation ladders of Arp 299 with the flux of each transition plotted as black asterisks with red error bars. In blue, green and yellow dotted lines we plot the PDR/PDR/mCDR (left), PDR/PDR/mPDR (center), and PDR/PDR/XDR (right) ISM phases with their filling factors. The composite model is plotted with a red solid line. The model H_2 density [log cm^{-3}], G/G_0 [log Habing flux] or F_X [log erg s^{-1} cm^{-2}], and percentage mechanical heating (α) are shown in the legend along with the relative contribution of each phase in terms of emission and column density.

burst galaxies, LIRGS and ULIRGS, whose data are publicly available (Lemaux et al. 2014). The drawback of Herschel is that it has very high spectral resolution but low spatial resolution. For instance, although NGC 253 and Arp 299 are galaxies in the local universe, their star-burst regions which are on the scale of 1 kpc are almost covered by a single beam of Herschel, see e.g. Figure-1 by Rosenberg et al. (2014a). Another such situation is the case of Mrk 231 by van der Werf et al. (2010), where although a myriad transitions of CO and H_2O were observed within the spectral window of Herschel, no spatial information was provided.

Having spatially and spectrally resolved observations is important in addressing the fact that the filling factors of the mPDR component of the models of NGC 253 and Arp 299 is less than one per cent. This indicates that the emission of the high-J transitions in the best fit models of both systems emanates from mechanically heated regions that are dense and localized. There is stronger evidence for this localization in the best fit model of Arp 299 compared to NGC253, where $\alpha = 0.25$ and 0.1 are required, respectively. The higher α for Arp 299 could be due to the fact that Arp 299 is under-going a merger, hence the heating budget of the "best-fit model" is more dominated by mechanical heating compared to that of NGC253. Further hints for localized mechanically heating regions are provided by Pon et al. (2014), where Herschel observations of the Perseus B1-East

5 region are used where a filling factor of 0.15% of shock heated regions by dissipated turbulence was estimated. This filling factor is close to the 0.1% filling factor of the best fit model of NGC253 and about 5 times smaller that of Arp299. Although Perseus is a molecular cloud and not a star-burst galaxy like Arp299 and NGC253, it is a star-forming region where the same kind of shock heating and dissipation could be occurring. Despite the fact that the estimated filling factors mentioned earlier are very close, their proximity could be a mere coincidence. Thus, it would be an interesting application of the grids of Chapter-3 to try to constrain the mechanical heating rate of Perseus using the observations by Pon et al. (2014) and compare it to the rate they estimate. Moreover, the method presented in Chapter-5 can be applied to the data as well as to try to estimate the density PDF and consequently the Mach number in Perseus. A thorough study can be achieved with the Atacama Large Millimeter Array (ALMA), where at least the same spectral resolution of Herschel is matched with much higher spatial resolution. Thus, the answer to the localization of the mechanically heated regions could be checked systematically without the need of multi-component modeling. In fact, where multiple PDR models were necessary to model the emission of a region covered by the large beam of Herschel, single PDR models would be needed to model the emission of the resolved regions by ALMA within the same region of that beam. Recent observations of the central kpc region of NGC 1614, a LIRG with $L_{IR} \sim 10^{11.65}$ $L_{\odot}$ (Xu et al. 2015), hint to localized bright CO(6-5) emission compared to CO(2-1) that requires cooler gas to be excited. Takano et al. (2014) observed the central region of NGC 1068 which hosts an AGN where they present emission of a few shock and dust related species. Such spatially resolved emission maps along with future observations by ALMA could be used to find a definitive diagnostic discriminating XDRs from mPDRs.

6.4.2 General improvements

- In the PDR models we assumed that the micro-turbulence line-width is fixed throughout the parameter space. This assumption was based on galaxy scale ISM simulations by Pelupessy & Papadopoulos (2009) (see Chapter-4), where a canonical value of 1 km/s was used also in computing the emission maps in Chapters-4 and 5. The main limitation was the excessive computing time required to interpolate over the emission grids to compute the emission maps. Although this was good enough for our qualitative analysis of the trends in the diagnostic line-ratios, the use of a micro-turbulence line-width derived from the mechanical heating or computed self-consistently from the modeled gas, e.g. from an SPH simulation, could be essential for an accurate study.

- We focused our attention to high-*J* transitions, showing that they could be considered good tracers of the physical conditions present in the mechanically heated regions of the ISM . However, low-*J* transitions like the case of CO(1-0) still need to be accurately modeled in the low density case since the molecular mass of clouds is usually inferred from the luminosity of CO(1-0). A detailed simulation of the Milky Way by Smith et al. (2014) estimates that almost 42% of the molecular mass is in gas not traced by CO, the so-called "CO-dark" gas. AREPO, which is a state of the art hydrodynamics code (Springel 2010), coupled with time dependent chemical evolution was used for that simulation, but very rough assumptions were done in the radiative transfer calculations. Namely, local thermal equilibrium was assumed in computing the CO(1-0) luminosity due to limited computational resources. A significant improvement over the LTE assumption would be able to produce the emission maps using the method presented in Chapter-3 where more accurate quantification of "CO-dark" gas can be achieved.

- Degeneracies between mPDR, CDRs and XDRs models: Meijerink et al. (2011) discuss the star-formation in environments with extreme mechanical feedback and cosmic ray rates with a comparison to X-ray dominated region. They find that OH^+, OH, H_2O^+, H_2O and H^3O^+ can be used as discriminants between XDRs and CDRs. Rosenberg et al. (2014b) find a similar behavior among XDR and CDR models where both perform poorly compared to mPDRs in fitting the molecular emission of Arp 299. It is worth noting that Rosenberg et al. (2014b) use CO, ^{13}CO , HCN, HNC and HCO^+ in their fitting procedure. On the other hand Meijerink et al. (2011) consider four models in their survey. Hence, it is interesting to increase the dimensionality of the grids by exploring possible ranges of X-ray heating and cosmic ray rates, in addition to considering the XDR – CDR discriminating species suggested by Meijerink et al. (2011), for the purpose of finding a unique diagnostic for these three types of regions.

- As an extension to the previous item, and to add more completeness to the modeling challenge, at the cost of further complexity, considering the ^{12}C / ^{13}C elemental ratio could have significant consequences on the outcome of the emission of the carbonaceous species. Ultimately for an accurate treatment of the huge minimization problem, i.e finding a best fit model with the proper statistical modeling, one must also consider the uncertainties involved in the chemical reaction constants and the Einstein coefficients and the collisional cross-sections used for computing the emission. An extensive review by Wakelam et al. (2010) discuss the challenges in modeling chemical networks one of which involves the propagation of uncertainties during the computations of the reaction rates. Clearly constructing grids, taking all the additional free parameters we mentioned, as was done in Chapter-2 and 3 is not a feasible solution. It is necessary to adopt sophisticated Monte-Carlo methods and smart-searching algorithms in finding a distinct diagnostic between XDRs, mPDRs and CDRs. In addition to such statistical modeling, it is also essential to have bigger data set against which the numerical modeling will be done. For example Papadopoulos et al. (2011) suggest that having more data such as multi-J transitions of CO, ^{13}CO and high density traces by ALMA could help find a unique diagnostic for CDRs.

- Needless to say, it is very important to have an accurate case study, a benchmark, against which the community can test the various numerical tools. The latest serious large scale comparison was done by Röllig et al. (2007). The "order-of-magnitude" discrepancy among the tools for a reduced PDR model is indicative of lack of a reference against which an astronomer can test his/her tools. A case relevant to this thesis would be having a basic benchmark to probe the influence of mechanical heating in a star-forming region; it is necessary to have a self-consistent time-dependent hydrodynamics code, coupled to a radiative transfer code that is able to resolve the shocks accurately as well as treat the chemistry accurately. It is not necessary for this benchmark case to solve the problem fully, but to capture the physics and chemistry well enough to establish a solid foundation upon which more sophistication can be added.