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# Mutual Effects of Radiation Field and Cosmic Rays on the Neutral and Molecular Interstellar Medium

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# Abstract

The photoelectric effect on dust grains is considered to be the dominant heating mechanism for the gas in the neutral and molecular interstellar medium. I investigate the effects of radiation fields with different intensities and colours on the photoelectric heating rate, and show that the near ultraviolet photons and optical photons has a significant contribution to the photoelectric heating rate in radiation fields in highly obscured regions in the interstellar medium. A new, self-consistent thermal and chemical model for the neutral and molecular interstellar medium is presented, and the mutual effects of radiation fields and cosmic rays on the thermal balance and chemistry of the gas are investigated. Including only the principle heating and cooling channels and the most observationally significant emission lines (e.g. CO pure rotational lines), the analytical approximations employed in the model makes it computationally fast and ideal to be incorporated into large-scale radiative transfer models for the propagation of starlight in galaxies. In addition, I show that the free electrons produced by cosmic ray ionisation of the interstellar gas particles lower the photoemission threshold of dust grains, thus boosting the photoelectric heating rate indirectly. Together with a simple semi-analytic spherical cloud model, the chemical model is applied to model the CO line emission in passive clouds in the nearby spiral galaxy NGC 628. The predicted CO line brightness is higher than the observed brightness by a factor of a few, and possible explanations for this overprediction are presented.

# Zusammenfassung

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Der photoelektrische Effekt auf Staubkörner wird als der dominierende Heizmechanismus für das Gas im neutralen und molekularen interstellaren Medium angesehen. Ich untersuche die Auswirkungen von Strahlungsfeldern unterschiedlicher Intensität und Farbe auf die photoelektrische Heizrate und zeige, dass die nahen ultravioletten Photonen und optischen Photonen einen signifikanten Beitrag zur photoelektrischen Heizrate in Strahlungsfeldern in stark verdunkelten Regionen im interstellaren Medium leisten. Ein neues, selbstkonsistentes thermisches und chemisches Modell für das neutrale und molekulare interstellare Medium wird vorgestellt, und die gegenseitigen Auswirkungen von Strahlungsfeldern und kosmischer Strahlung auf den Wärmehaushalt und die Chemie des Gases werden untersucht. Da das Modell nur die wichtigsten Heiz- und Kühlkanäle und die wichtigsten Emissionslinien (z. B. reine CO-Rotationslinien) enthält, ist es dank der analytischen Näherungen, die in dem Modell verwendet werden, rechnerisch schnell und ideal für die Einbeziehung in großmaßstäbliche Strahlungstransportmodelle für die Ausbreitung von Sternenlicht in Galaxien. Darüber hinaus zeige ich, dass die freien Elektronen, die durch die Ionisierung der interstellaren Gasteilchen durch die kosmische Strahlung erzeugt werden, die Photoemissionsschwelle der Staubkörner herabsetzen und damit indirekt die photoelektrische Heizrate erhöhen. Zusammen mit einem einfachen semi-analytischen sphärischen Wolkenmodell wird das chemische Modell angewandt, um die CO-Linienemission in passiven Wolken in der nahen Spiralgalaxie NGC 628 zu modellieren. Die vorhergesagte Helligkeit der CO-Linie ist um einen Faktor höher als die beobachtete Helligkeit, und es werden mögliche Erklärungen für diese Übervorhersage vorgestellt.

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This work made use of the following software packages: matplotlib (Hunter, 2007), numpy (Harris et al., 2020), and python (Van Rossum and Drake, 2009). Software citation information aggregated using The Software Citation Station (Wagg and Broekgaarden, 2024; Wagg and Broekgaarden, 2024).

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# **List of Abbreviations**

| ALMA           | Atacama Large Millimeter/Submillimeter Array                         |
|----------------|--|
| СМВ            | Cosmic Microwave Background  |
| CMZ            | Central Molecular Zone   |
| CNM            | Cold Neutral Medium  |
| <b>CR</b> (s)  | Cosmic Ray(s)  |
| CRIR           | Cosmic Ray Ionisation Rate   |
| FIR            | Far Infrared   |
| FUV            | Far Ultraviolet  |
| <b>GMC</b> (s) | Giant Molecular Cloud(s)   |
| HERACLES       | Heterodyne Receiver Array CO Line Extragalactic Survey               |
| ISM            | Interstellar Medium  |
| ISRF           | Interstellar Radiation Field   |
| JWST           | James Webb Space Telescope   |
| KINGFISH       | Key Insights on Nearby Galaxies: a Far-Infrared Survey with Herschel |
| MIPS           | Multiband Imaging Photometer (Spitzer)                               |
| MIR            | Mid Infrared   |
| NGC            | New General Catalogue of Nebulae and Clusters of Stars               |
| NIR            | Near Infrared  |
| NUV            | Near Ultraviolet   |
| PAH(s)         | Polycyclic Aromatic Hydrocarbon(s)                                   |
| <b>PDR</b> (s) | Photodissociation Region(s)  |
| PE             | Photoelectric  |
| PHANGS         | Physics at High Angular resolution in Nearby Galaxies                |
|                |  |

# RTRadiative TransferTHINGSThe H I Nearby Galaxies SurveySEDSpectral Energy DistributionWIMWarm Ionised MediumWNMWarm Neutral Medium

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# **Physical Constants**

| speed of light                  | $c = 2.99792458 \times 10^{10} \text{ cm s}^{-1} \text{ (exact)}$   |
|---------------------------------|---|
| elementary charge               | $e = 4.8032 \times 10^{-10} \text{ cm}^{3/2} \text{ g}^{1/2} \text{ s}^{-1}$  |
| Newton's gravitational constant | $G = 6.6743 \times 10^{-11} \text{ cm}^3 \text{ g}^{-1} \text{ s}^{-2}$   |
| Planck's constant               | $h = 6.6261 \times 10^{-27} \text{ cm}^2 \text{ g s}^{-1} = 6.6261 \times 10^{-27} \text{ erg s}$                             |
| Boltzmann's constant            | $k_{\rm B} = 1.3807 \times 10^{-16} \text{ cm}^2 \text{ g s}^{-2} \text{ K}^{-1} = 1.3807 \times 10^{-16} \text{ erg K}^{-1}$ |
| electron mass                   | $m_{\rm e} = 9.1094 \times 10^{-28} \text{ g} = 0.511 \text{ MeV}/c^2$  |
| proton mass                     | $m_{\rm p} = 1.6726 \times 10^{-24} \text{ g} = 938.3 \text{ MeV}/c^2$  |
| Stephan-Boltzmann constant      | $\sigma_{\rm SB} = 5.6704 	imes 10^{-5} {\rm ~g~s^{-3}~K^{-4}}$   |

# **List of Symbols**

## List of most common or self-defined symbols used in this thesis

| а                  | radius of dust grain   | Å or cm  |  |
|--------------------|--|--|--|
| В                  | magnetic field strength  | μG   |  |
| col <sub>FUV</sub> | "colour" of FUV radiation field (Eqn. 2.31)                                |  |  |
| EA                 | electron affinity  | eV   |  |
| $f_{\rm H_2}$      | molecular fraction   |  |  |
| Fgr                | fraction of metals in grains   |  |  |
| $G_0$              | intensity of FUV radiation field in Habing units                           |  |  |
| $G_{\rm FUV}$      | intensity of FUV radiation field relative to Mathis et al. (1983) ISRF     |  |  |
| G <sub>ini</sub>   | scaling factor of Mathis et al. (1983) ISRF before extinction (Eqn. 2.23)  |  |  |
| G <sub>opt</sub>   | intensity of optical radiation field relative to Mathis et al. (1983) ISRF |  |  |
| G <sub>NUV</sub>   | intensity of NUV radiation field relative to Mathis et al. (1983) ISRF     |  |  |
| IP                 | ionisation potential   | eV   |  |
| j                  | line emissivity  | ${\rm erg}~{\rm cm}^{-3}~{\rm s}^{-1}~{\rm sr}^{-2}$ |  |
| k                  | rate coefficient of chemical reaction                                      | ${\rm cm}^{-3}~{\rm s}^{-1}~{\rm or}~{\rm s}^{-1}$   |  |
| п                  | gas number density   | $\mathrm{cm}^{-3}$                                   |  |
| n <sub>e</sub>     | electron density   | $\mathrm{cm}^{-3}$                                   |  |
| $n_{\rm H}$        | number density of hydrogen nuclei  | $\mathrm{cm}^{-3}$                                   |  |
| n <sub>α</sub>     | number density of species $\alpha$   | $\mathrm{cm}^{-3}$                                   |  |
| $N_{\mathrm{H}}$   | column density of hydrogen nuclei  | $\mathrm{cm}^{-2}$                                   |  |
| $P_{\rm CR}$       | cosmic ray pressure  | $k_{\rm B}{\rm K}{\rm cm}^{-3}$                      |  |
| P <sub>mag</sub>   | magnetic pressure  | $k_{\rm B}{\rm K}{\rm cm}^{-3}$                      |  |

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| P <sub>therm</sub>                    | thermal pressure   | $k_{\rm B}{ m K}{ m cm}^{-3}$           |
|---------------------------------------|--|---|
| $Q_{abs}$                             | absorption coefficient (of dust grains)  |   |
| s <sub>e</sub>                        | sticking coefficient for electrons   |   |
| $s_{\mathrm{H}}$                      | sticking coefficient for hydrogen atoms  |   |
| Т                                     | gas temperature  | К                                       |
| T <sub>d</sub>                        | temperature of dust grain  | К                                       |
| $u_{\nu}$                             | specific energy density (of radiation field)   | ${\rm erg}~{\rm cm}^{-3}~{\rm Hz}^{-1}$ |
| $x_{\alpha}$                          | abundance of species $\alpha$ relative to hydrogen   |   |
| X <sub>CO</sub>                       | CO-to-H <sub>2</sub> conversion factor   | $cm^{-2}(K km/s)^{-1}$                  |
| $W(\nu)$                              | a function to form new ISRFs (Sec. 2.5.2)  |   |
| y                                     | photoelectric yield  |   |
| Ζ                                     | electric charge of dust grains/particles   | е                                       |
| Z'                                    | metallicity of the ISM (relative to solar metallicity)                                     |   |
| $\epsilon_{ m H_2}$                   | formation efficiency of H <sub>2</sub>   |   |
| $\gamma$                              | grain charging parameter   | $K^{1/2} cm^3$                          |
| $\gamma'$                             | modified grain charging parameter (Sec. 2.5.4)   | $K^{1/2} cm^3$                          |
| Γα                                    | volumetric gas heating rate due to process $\alpha$  | ${\rm erg}~{\rm cm}^{-3}~{\rm s}^{-1}$  |
| λ                                     | photon wavelength  | Å or µm                                 |
| $\Lambda_{\alpha}$                    | volumetric gas cooling rate due to process $\alpha$  | ${\rm erg}~{\rm cm}^{-3}~{\rm s}^{-1}$  |
| ρ                                     | gas mass density   | ${\rm g}~{\rm cm}^{-3}$                 |
| ν                                     | photon frequency   | Hz                                      |
| $\nu_{\rm pet}$                       | photoemission threshold frequency  | Hz                                      |
| $\sigma_v$                            | velocity dispersion  | $\rm km~s^{-1}$                         |
| $	au_{ m B}$                          | B-band optical depth   |   |
| $\zeta_{\rm H}$                       | total cosmic ray ionisation rate of hydrogen (including H $\ensuremath{\text{I}}$ and H_2) | $s^{-1}$                                |
| $\zeta_{\rm H{\scriptscriptstyle I}}$ | total cosmic ray ionisation rate of atomic hydrogen  | $s^{-1}$                                |
| $\zeta_{\rm H_2}$                     | total cosmic ray ionisation rate of H <sub>2</sub>   | $s^{-1}$                                |
| $\zeta_{\rm p}$                       | primary cosmic ray ionisation rate of atomic hydrogen                                      | $s^{-1}$                                |

# Chapter 1

# Introduction

## 1.1 Overview of the interstellar medium

The interstellar medium (ISM), the space between the stars within the Milky Way and other spiral galaxies, is not just empty space, but contains gas, dust, photons, cosmic rays and magnetic fields. The gas in the ISM is mainly composed of atomic hydrogen (H I), first observed via its 21-cm hyperfine transition (spin reversal) line by Ewen and Purcell in 1951 (Oort (1955)), and also molecular hydrogen (H<sub>2</sub>). Apart from obscuring starlight with the dust it contains, the ISM is also the birthplace of stars. Larson (1969) then found the first robust theoretical foundation for the collapse of molecular clouds to form stars. As will be explained in the following sections, different components of the ISM interact with each other in a complex way and affect the distribution of interstellar gas in galaxies.

There are mutual interactions among the constituents in the interstellar medium, as shown in Figure 1.1.



FIGURE 1.1: Interactions between the constituents of the interstellar medium (and the intergalactic medium)

## 1.2 Interstellar gas

#### 1.2.1 Phases of the interstellar medium

Commonly, 5 distinct phases in the interstellar medium are identified, as shown in Table 1.1. According to the classification in the reivew by Snow and McCall (2006), molecular clouds can be further divided into diffuse molecular clouds (where the fraction of gas-phase carbon in C<sup>+</sup>,  $f_{C^+}$ , is greater than 0.5), translucent clouds (where  $f_{C^+} < 0.5$  and  $f_{CO} < 0.9$ ), and dense molecular clouds (where  $f_{CO} > 0.9$ ).

| Component                 | Temperature (K) | Density (cm <sup>-3</sup> ) | Fractional ionisation |
|---------------------------|-----------------|-----------------------------|-----------------------|
| Molecular clouds          | 10–20           | > 10 <sup>2</sup>           | $< 10^{-6}$           |
| Cold neutral medium (CNM) | 50–100          | 20–50                       | $\sim 10^{-4}$        |
| Warm neutral medium (WNM) | 6000-10000      | 0.2–0.5                     | $\sim 0.1$            |
| Warm ionised medium (WIM) | $\sim 8000$     | 0.2–0.5                     | 1.0                   |
| Hot ionised medium (HIM)  | $\sim 10^{6}$   | $\sim 10^{-2}$              | 1.0                   |

TABLE 1.1: Phases of the interstellar medium (Adapted from Klessen and Glover (2016))

In this thesis, I will focus on the cooler components of the interstellar medium, namely the cold neutral medium (CNM) and molecular clouds. These carry by far the large majority of molecular gas mass in the ISM, and a sizeable fraction of the neutral hydrogen gas.

#### **1.2.2** Problems with observing the H<sub>2</sub> gas

Hydrogen (in atomic or molecular form) is the most abundant element in interstellar gas. Atomic hydrogen (H I) dominates the diffuse interstellar medium, while molecular hydrogen (H<sub>2</sub>) dominates the denser regions of the interstellar medium, including molecular clouds. H I can be directly observed by its 21-cm hyperfine transition line. Having large spacings between its rotational levels and being a light symmetric molecule, H<sub>2</sub> does not radiate efficiently at low temperatures so it is practically invisible in the cold molecular medium. Therefore, we need tracers to detect and measure H<sub>2</sub> gas. Carbon monoxide (CO) is widely used as a tracer of H<sub>2</sub> as it offers many advantages over other molecular tracers when probing the molecular ISM (Bolatto, Wolfire, and Leroy (2013)). It is the second most abundant molecule in the molecular ISM, after H<sub>2</sub>. Furthermore, the first excited rotational energy state of CO is only 5.5 K above the ground state, so even cold (T < 10 K) interstellar molecular gas emits the CO  $J = 1 \rightarrow 0$  line. At a wavelength of 2.6 mm, the CO  $J = 1 \rightarrow 0$ line falls in a fairly transparent window in the terrestrial atmosphere.

#### **1.2.3** CO as a tracer of $H_2$ gas

The relationship between the hydrogen surface density  $N(H_2)$  and the observed intensity of <sup>12</sup>CO  $J = 1 \rightarrow 0$  line emission  $W_{CO}$  is often quantified by the  $X_{CO}$  factor:

$$X_{\rm CO} \equiv \frac{N(\rm H_2)}{W_{\rm CO}} \tag{1.1}$$

where  $W_{CO} \equiv \int T_B(v) dv$  is the brightness temperature of the CO line integrated over the velocity width of the cloud (see e.g. Heyer and Dame (2015)). Observations have determined that  $X_{CO} = (1.8 \pm 0.3) \times 10^{20} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1}$  for galactic latitude  $b > |5^\circ|$  in the Milky Way (Dame, Hartmann, and Thaddeus (2001)). However, there is empirical evidence that the  $X_{CO}$  factor depends on environmental factors such as gas metallicity, surface density and strength of the interstellar radiation field (Bolatto, Wolfire, and Leroy (2013)), all factors that can vary within and between galaxies by an order of magnitude or more.

In the cold neutral medium, gas-phase carbon in the interstellar medium is mainly contained in  $C^+$ . As the optical depth becomes higher and UV photons become more sparse, most  $C^+$  becomes atomic carbon (C) by recombining with electrons. This occurs in the "translucent" region in a molecular cloud (Snow and McCall (2006)).

In the denser regions of a molecular cloud where the UV flux is very low, most gasphase carbon is contained in CO (see e.g. Nelson and Langer (1999), Keto and Caselli (2008), Glover et al. (2010)). Here, usually most of the hydrogen nuclei are contained in H<sub>2</sub>.

#### **1.2.4** Molecular clouds and star formation

It is widely believed that cold  $H_2$  gas is required for stars to form; however, recent studies suggest that atomic gas (H I gas) can also form stars as efficiently as molecular gas (Glover and Clark (2012)).

In self-gravitating molecular clouds, the thermal pressure is the main force counteracting the force of gravity. According to the simple theory of Larson (1969), once the mass of the cloud reaches a critical value, the thermal pressure can no longer overcome the pulling force of gravity, and the cloud collapses. Eventually, both the density and the temperature of the cloud becomes high enough so that a protostar is formed. Thermal pressure becomes very important in the small scale of pre-stellar cloud cores.

In 1981, Larson analysed observational data on molecular clouds and discovered that turbulence pressure is an important factor in providing the support of molecular clouds against gravity (Larson (1981)). In the scale of giant molecular clouds (GMCs), both magnetic pressure and turbulence pressure are more important (Larson (2003)). The effects of magnetic pressure on the thermodynamic state of neutral and molecular clouds are discussed in Chapter 4. The cloud model introduced in Chapter 5 takes turbulence into account in the form of velocity dispersion.

#### 1.2.5 Heating and cooling of interstellar gas

Photoelectric (PE) heating has long been postulated to be the dominant heating mechanism in diffuse clouds (e.g. de Jong (1977)), especially in regions with strong UV illumination and/or low cosmic ray flux. In principle, PE heating can be manifested in two ways: (i) PE heating on dust grains, and (ii) PE heating on metal atoms/ions such as C I, which is generally referred to as photoionisation. In the first case, photoelectrons are ejected from a dust grain after a photon with high enough energy hits the dust grain. In the second case, photoelectrons are ejected after a UV photon hits a single metal atom/ion (i.e. a photoionisation). In general, the PE heating effect on dust grains is often stronger than the heating effect from metal atoms, since dust grains receive a broad band response to photons whereas atoms only absorb UV photons in a narrow band. Figure 1.2, taken from Tielens (2005), shows that the PE heating on dust grains (labelled "pe") dominate over the PE heating from C I (labelled "CI"). Unless otherwise stated, "PE heating" in this thesis refers to the PE

heating on dust grains.

Figure 1.2 also shows the dominating effect of PE heating in diffuse clouds. In dense molecular clouds with very weak UV flux due to high optical depth, however, the heating due to cosmic rays can exceed or even dominate over PE heating. In the latter case, cosmic rays, instead of photons, control the overall thermal state of the interstellar gas. In Chapter 3, the conditions in which cosmic ray heating dominates over PE heating are investigated.



FIGURE 1.2: Heating processes in diffuse clouds in the local ISRF with a gas temperature of 100 K and an electron fraction of  $1.4 \times 10^{-4}$ . The plot shows heating due to grain photoelectric effect (pe), cosmic rays (CR), photoionisation of neutral carbon (CI) and X-rays. Figure from Tielens (2005), reproduced with permission of The Licensor through PLSclear.

In principle, extreme ultraviolet photons (EUV) can also heat up the gas in the ISM. These are the photons that are more energetic than the ionisation energy of atomic hydrogen, 13.6 eV, corresponding to a wavelength of 912 Å, and this is a very dominant heating process in H II regions. However, since I focus on the general ISM regions away from energetic sources such as O stars, most photons with wavelengths shorter than 912 Å are consumed by the ionisation of H I from the ground state. Hence, very few EUV photons, if any, remain in the ISRF. Therefore, gas heating from EUV photons are not considered in this thesis.

The gas heating is balanced by gas cooling in equilibrium state. The fine structure 158  $\mu$ m line emission of C II is the dominant cooling mechanism in diffuse clouds (see e.g. Lagache, Cousin, and Chatzikos (2018)), as it is often the main form of carbon in these low-density regions, and carbon can be ionised by FUV photons, unlike

e.g. oxygen. The rotation lines of CO are often the most important cooling mechanism in molecular clouds (Neufeld, Lepp, and Melnick (1995)).

Other important coolants in the (cold) neutral interstellar medium include OI and CI, which are incorporated in the chemical model that will be discussed in Chapter 3.

## 1.3 The role of interstellar dust

This section describes the role of interstellar dust in the ISM - attenuating starlight, as the site for photoelectric heating, and as a catalyst for the formation of  $H_2$ .

## 1.3.1 Attenuation of starlight

Interstellar dust was discovered around 1930 (Trumpler (1930)) when astronomers noticed that the light from distant stars suffers from extinction by the intervening material. Interstellar dust grains scatter and absorb starlight. The combined effects of scattering and absorption is called extinction. Since dust grains absorb FUV photons more strongly than optical photons (see Figure 1.3), the colour of starlight after passing through the interstellar medium becomes redder. Therefore, the selective extinction by interstellar dust is also called reddening. This effect leads to the phenomenon that the ISRF in the interior of a molecular cloud is both weaker and redder than the ISRF at the surface of the molecular cloud. As will be discussed in future chapters, the colour of ISRF has an important effect on the PE heating of the gas, and ultimately, the thermodynamic structure of the cloud.


FIGURE 1.3: Absorption coefficient of neutral polyaromatic hydrocarbon (PAH) dust grains of different sizes. *a* is the radius of the dust grain. Data obtained from Weingartner and Draine (2001a).

#### **1.3.2** Photoelectric heating on dust grains

As mentioned already in Section 1.2.5, apart from obscuring starlight, interstellar dust also plays a role in the heating of interstellar gas via the PE effect on dust grains. After ultraviolet (UV)/optical photons from starlight collide with a dust grain, a photoelectron, carrying part of the photon energy, is ejected from the grain if its kinetic energy is high enough to overcome the energy barrier. The details will be discussed in Chapter 2.

#### **1.3.3** As a catalyst for the formation of H<sub>2</sub>

In the cold interstellar medium ( $T \le 100$  K), the formation rate of molecular hydrogen from the collision of two hydrogen atoms is typically very low. So how is H<sub>2</sub> able to form in the cold ISM? It was proposed that the interstellar dust grains actually act as catalytic sites for the formation of H<sub>2</sub> (Gould and Salpeter (1963)). Basically, two hydrogen atoms combine to form a hydrogen molecule after they are adsorbed onto a dust grain. This process is able to account for the observed H<sub>2</sub> formation rate in the ISM (Jura (1975)).

# 1.4 Interstellar radiation field

The UV/optical part (0.09  $\mu$ m <  $\lambda$  < 0.7  $\mu$ m) of the interstellar radiation field (ISRF) is mainly contributed by starlight photons, while the near infrared/mid-infrared section (5  $\mu$ m  $\lesssim \lambda \lesssim 100 \mu$ m) is dominated by emission of interstellar dust. In the microwave regime ( $\lambda \gtrsim 0.3$  mm), the ISRF is dominated by photons from the cosmic microwave background radiation. Figure 1.4 shows the spectral energy distribution (SED) of the ISRF of the Milky Way in the solar neighbourhood due to direct and dust-reradiated starlight (Popescu et al. (2017)).



FIGURE 1.4: Radiative transfer model prediction of the SED of the local ISRF in the Milky Way due to direct and dust-reradiated starlight. The squares are the sampling points of the radiative transfer model for the direct stellar light, while the red triangles are measurements of direct starlight from Henry, Anderson, and Fastie (1980) and Witt and Johnson (1973). Figure reproduced from Popescu et al. (2017).

#### 1.4.1 Habing (1968) radiation field

Habing (1968) was one of the earliest to come up with an estimate of the intensity of the ISRF at the solar neighbourhood due to UV starlight. His estimate of the strength of the FUV average interstellar radiation,  $1.2 \times 10^{-4}$  erg cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup>, is often used to express the strength of the interstellar FUV radiation field:

$$1 G_0 = 1.2 \times 10^{-4} \operatorname{erg} \operatorname{cm}^{-2} \operatorname{s}^{-1} \operatorname{sr}^{-1}.$$
 (1.2)

The integrated energy density in Habing's radiation field between 912 Å and 2400 Å is  $5.6 \times 10^{-14}$  erg cm<sup>-3</sup>. The Habing field is commonly used as a unit for expressing the intensity of the ISRF.

## 1.5 Cosmic rays

#### 1.5.1 Cosmic ray ionisation

Cosmic rays (CRs) are energetic particles traversing large distances in galaxies. The exact origin of the production of CRs is unknown, although it has been proposed that CRs originate from the shocks of supernova remnants (Hayawaka, Ito, and Terashima (1958)). CR particles consist of mostly protons, but also electrons and heavier nuclei. The energy in CRs are dominated by hadrons, rather than electrons. CR particles, especially low energy CR particles (E < 1 GeV), are crucial agents in the ionisation of the interstellar gas. The electrons produced during the ionisation of gas particles greatly influence the chemistry of the interstellar gas. Figure 1.5 shows the CR spectrum as measured on Earth.



FIGURE 1.5: CR spectrum as measured on Earth, with data points obtained from various experiments. Figure reproduced with permission from Margiotta (2014). © IOP Publishing

#### 1.5.2 Cosmic ray heating

As already mentioned, CRs are also responsible for heating up the interstellar gas indirectly through ionising the gas particles. The kinetic energy in the CR particles is transferred to the ejected electrons during the ionisation, which distribute its kinetic energy by thermalising with the gas particles. Although CR heating is not believed to be as important as PE heating in the relatively unobscured parts of the diffuse ISM, CR heating may become important compared to PE heating in highly obscured regions with high densities, such as the cores of molecular clouds. One of the goals of this thesis is to attempt to quantify the conditions in which CR heating takes over PE heating as the dominant heating mechanism of interstellar gas.

# **1.6** Link of PE heating to the gas cycle

The "gas cycle" in galaxies begins when diffuse atomic clouds slowly collapse into molecular clouds, which further collapse into protostars when the gas density is high enough. As stars evolve, they eject hot ionised gas back to the interstellar medium gradually (e.g. through stellar winds) or catastrophically (e.g. as supernova explosions). The hot ionised gas then slowly cools by thermal emission into cold H<sub>I</sub> gas, which slowly collapse into molecular clouds. As these neutral clouds and molecular clouds are the precursor of stars, understanding them can help us gain better insight into star formation and galaxy evolution. In particular, because the timescale for the cooling of diffuse gas is longer than that for dense gas, the main bottleneck in the gas cycle may well be the formation and collapse of diffuse clouds. Given that, in diffuse clouds, gas heating is postulated to be dominated by PE heating, PE heating may be a fundamental process controlling the gas cycle. Figure 1.6 shows a sketch of the gas cycle in galaxies.



FIGURE 1.6: A sketch of the gas cycle in galaxies. The species in red text are the major observational tracer(s) of the corresponding stage in the gas cycle. Reproduced from Kuleza et al. (2013).

### **1.7** The need for a new PE heating model

In many hydrodynamic codes or photodissociation region models, e.g. the Meudon PDR code (Le Petit et al. (2006)), the only parameter characterising the ISRF incident on the surface of the cloud is a single scalar quantity, either in terms of the Habing field  $G_0$ , or in units of the Draine (1978) ISRF ( $\chi$ ). For efficiency, hydrodynamical simulations often use the Bakes and Tielens (1994) formulation of photoelectric heating. This formulation uses the gas temperature, the electron density and one single parameter to characterise the ISRF,  $G_0$ . As will be demonstrated in Chapter 2, IS-RFs with the same integrated energy density but with different colours can result in widely different photoelectric heating rates. Therefore, when considering the wide range of colours of ISRFs in obscured regions, including clouds, there is a need for a new PE heating model that can take both the intensity and the colour of the ISRF into account. This PE heating model is the topic of the next chapter.

# Chapter 2

# The photoelectric heating model

# 2.1 The photoelectric effect on interstellar dust grains

As discussed in Chapter 1, the photoelectric ejection of electrons from interstellar dust grains is widely considered to be an important heating source for the interstellar medium (Watson (1972), de Jong (1977)). When a dust grain absorbs a photon from the interstellar radiation field, if the incident photon is sufficiently energetic, an ionisation process leading to the ejection of an electron may occur. A fraction of the absorbed photon energy is dissipated by inelastic collisions of the excited electron with the carbon atoms in the grain as the excited electron scatters through the grain material on its way to the grain surface. Some energy is required to overcome the Coulomb barrier if the grain is now positively charged. The electron will emerge from the grain with some kinetic energy, which will be converted into thermal energy of the gas via inelastic collisions. In this way, the photon energy contained within the interstellar radiation field is transferred to the gas particles in the ISM, thereby heating the gas. Figure 2.1 shows a simplified schematic of the photoelectric heating mechanism.

As the photoelectron has to overcome the Coulomb potential of the grain to escape from the grain, the minimum energy required for a photon to initiate the photoelectric process greatly depends on the ionisation potential of the grain. If the grain is positively charged, the electrostatic force between the grain and the electron would be higher than if the grain is electrically neutral. On the other hand, grains that are negatively charged can "push" the electron away with their repulsive electrostatic force, essentially giving the electron an extra boost. Photons that do not possess energy higher than the ionisation potential of the grain cannot initiate the photoelectric effect. As will be discussed in the next sections, the charge states of interstellar dust grains greatly influence the photoelectric heating efficiency.



FIGURE 2.1: A schematic of the photoelectric heating mechanism. Note that in this thesis the PAH molecules will be treated as small spherical grains as displayed in the right diagram. Figure from Tielens (2005), reproduced with permission of The Licensor through PLSclear.

# 2.2 Historical perspective

The photoelectric emission from interstellar dust grains was investigated as early as 1948 (Spitzer (1948)). However, no information was available for the galactic UV starlight at that time, nor were laboratory data for photoemission available for photon energies greater than  $\sim 10$  eV (Watson (1972)). This section provides an overview of the proposed models of photoelectric emission from dust grains, starting from the Watson (1972) model.

#### 2.2.1 Watson (1972) model

In 1972, equipped with laboratory measurements of photoemission on solids, William Watson formulated a simple model for photoelectric heating on interstellar dust grains (Watson (1972)). He assumed a simple analytical model for the average energy of an ejected electron and only considered UV photons with energies between 10.1 eV and 13.6 eV. He obtained a photoelectric heating rate per hydrogen atom of

$$\Gamma_{\rm pe} = y \, Q_{\rm abs} \frac{n_{\rm d} \sigma_{\rm d}}{n_{\rm H}} \, F_{\rm eV} \, \frac{(3.5 - V_0)^2}{2} \tag{2.1}$$

where  $Q_{abs}$  is the absorption coefficient of the dust grain,  $n_d$  is the number density of dust grains,  $\sigma_d$  is the surface area of a dust grain,  $V_0$  is the positive electric potential for photoemission in volts,  $n_H$  is the hydrogen nuclei density (in either H<sub>I</sub> or H<sub>2</sub>) and  $F_{eV}$  is the photon flux per eV. Watson assumed that the photoelectric yield y = 0.1. The photoelectric yield is the probability that a photon with a

certain energy successfully leads to the ejection of an photoelectron, after the photon is absorbed by the grain (Weingartner and Draine (2001b)) (some authors use the term "photoelectric emission efficiency" instead of photoelectric yield). In later models (e.g. Weingartner and Draine (2001b) model), the dependence of *y* on grain size, grain charge and grain composition was explicitly calculated. It is obvious that the photoelectric heating rate is simply proportional to the photon flux, and while Watson included the consideration of the electric charge of dust grains, it is simply incorporated by the parameter  $V_0$ . Watson also assumed that the sticking coefficient of electrons  $s_e$  is 1, which is not shown in Equation 2.1.  $s_e$  is the probability that an electron sticks to the surface of a grain after colliding with it. This is essential to the collisional charging of grains, and this parameter was implemented more properly in Weingartner and Draine (2001b).

#### 2.2.2 de Jong (1977) model

Teije de Jong published his photoelectric heating model in 1977, five years after Watson published his model. de Jong's model formulated grain charging in a more sophisticated way that bears resemblance to the analytical approximation in Bakes and Tielens (1994), which will be discussed in the next section. In essence, grain charging in de Jong's model is a function of the gas temperature *T* and the electron density  $n_{\rm e}$ . The volumetric photoelectric heating rate is

$$\Gamma_{\rm pe} = 7.5 \times 10^{-25} \, y \chi n \left( \frac{1 - x_{\rm d}}{x_{\rm d} + 2\gamma_{\rm dJ}} \right)^2 \, \rm erg \, \rm cm^{-3} \, \rm s^{-1} \tag{2.2}$$

where

$$\gamma_{\rm dJ} \equiv \left(\frac{km_{\rm e}}{8}\right)^{1/2} \frac{c^2}{h^2 \nu_{\rm H}^3} \frac{y u_{\lambda} T^{1/2}}{n_{\rm e}} = 2.9 \times 10^{-4} \left(\frac{y \chi \sqrt{T}}{n_{\rm e}}\right)$$
(2.3)

is the "charging parameter" of dust grains in de Jong's model. In Equation 2.2,  $x_d \equiv v_d/v_H$ ,  $v_H$  is the frequency of the Lyman limit (912 Å),  $v_d$  is the photoelectric threshold energy of the bulk dust material,  $hv_H$  is the energy required for an electron in the ground state of a hydrogen atom to escape from the electric potential of the proton that confines it,  $\chi$  represents the strength of the ISRF in units of the Draine (1978) ISRF, n is the gas number density in cm<sup>-3</sup>,  $n_e$  is the electron density in cm<sup>-3</sup>, and T is the gas temperature in K.

de Jong adopted  $hv_d = 10$  eV for graphite and silicate grains. He used y = 0.01 for graphite and y = 0.1 for silicates. Using constant values for y, then, the PE heating rate only depends on  $\chi$ , n,  $n_e$  and T. This is a simple formulation of PE heating that only takes the overall strength of the ISRF ( $\chi$ ) into account. In de Jong's paper, it was already mentioned that the PE heating rate is extremely sensitive to the value of the photoemission threshold of the dust material. However, this point was not

quantitatively demonstrated in his paper.

#### 2.2.3 Bakes and Tielens (1994) model

Compared to de Jong's model, the PE heating model of Bakes and Tielens (1994) treated the photoemission threshold in a more sophisticated manner. They started with the ionisation potential of a dust grain, which is a function of the grain charge and the number of carbon atoms in the dust grain. The formula for the ionisation potential of spherical grains employed by Bakes and Tielens is:

IP = 4.4 + 
$$\left(Z + \frac{1}{2}\right) \frac{11.1}{N_{\rm C}^{1/3}} \,{\rm eV},$$
 (2.4)

where Z is the grain charge and  $N_{\rm C}$  is the number of carbon atoms in the grain.

When determining the grain charge, Bakes and Tielens considered the equilibrium charge state by balancing the processes that change the charge state of a grain. Collisional charging of positive ions with grains and the emission of photoelectrons increases the grain charge by 1, and collisional charging of electrons with grains decreases the grain charge by 1. To calculate the collisional charging rates, Bakes and Tielens followed the "elegant study" of Draine and Sutin (1987), which will also be employed by the Weingartner and Draine (2001b) model later. Essentially, Bakes and Tielens considered the charge distribution of grains as a function of grain size and gas temperature.

Bakes and Tielens adopted the Mathis-Rumpl-Nordsieck (MRN) grain size distribution (Mathis, Rumpl, and Nordsieck (1977)):

$$\frac{\mathrm{d}n}{\mathrm{d}a} = a^{-3.5} \quad \text{for } a_{\min} \le a \le a_{\max}, \tag{2.5}$$

where  $a_{\min} = 3.1$  Å and  $a_{\max} = 1 \ \mu m$ . The MRN grain size distribution was obtained by fitting the interstellar extinction from infrared ( $\lambda = 1 \ \mu m$ ) to ultraviolet wavelengths.

By fitting a function to their calculated PE heating rates, Bakes and Tielens formulated a simple analytical expression for the PE heating rate in terms of  $G_0$ , T and  $n_e$ :

$$\Gamma_{\rm pe}(\gamma) = 1 \times 10^{-24} \epsilon(\gamma) \,\mathrm{erg} \,\mathrm{cm}^{-3} \,\mathrm{s}^{-1}, \tag{2.6}$$

$$\epsilon(\gamma) = \frac{4.87 \times 10^{-2}}{1 + 4 \times 10^{-3} \gamma^{0.73}} + \frac{3.65 \times 10^{-2} (T/10^4 \text{ K})^{0.7}}{1 + 2 \times 10^{-4} \gamma},$$
(2.7)

where  $\gamma \equiv G_0 \sqrt{T}/n_e$  is the grain charging parameter and  $G_0$  is the intensity of the ISRF in Habing units. Figure 2.2 shows the PE heating efficiency versus the grain

charging parameter.



FIGURE 2.2: Photoelectric heating efficiency versus grain charging parameter, as formulated by Bakes & Tielens (1994). The lines essentially overlap, showing that the dependence of the PE heating efficiency on the grain charging parameter is insensitive to changes of the gas temperature.

Although Bakes and Tielens' simple analytical expression compares well with their numerically calculated heating efficiency values, the ISRF is still expressed in a single scalar parameter  $G_0$ . This will be shown to be inadequate in capturing the effects of radiation fields with different 'colours', as shown in Section 2.4.2.

# 2.3 Weingartner & Draine (2001) model

Building on the previous models, the Weingartner and Draine (2001b) model (WD01b) is the most sophisticated model for PE heating to date. All later calculations of the thesis will be done entirely following this model for PE heating, except an omission of a term in the grain charging balance equation, which will be discussed in Section 2.3.7. The following subsections give an overview of the WD01b PE heating model. The full details of the model are given in Appendix A.

#### 2.3.1 Ionisation potential and electron affinity

In the WD01b PE heating model, the valence band ionisation potential  $IP_V$ , defined as the difference in energy between infinity and the top of the valence band (Weingartner and Draine (2001b)), is given by

$$IP_{V}(Z) = W + \left(Z + \frac{1}{2}\right)\frac{e^{2}}{a} + (Z + 2)\frac{e^{2}}{a}\frac{0.3 \text{ Å}}{a},$$
(2.8)

with the graphite work function W = 4.4 eV and *a* is the radius of the grain<sup>1</sup>. This value is taken to be the work function for carbonaceous grains. For silicate grains, W = 8.0 eV. Equation 2.8 is used to calculate IP<sub>V</sub> for both carbonaceous and silicate grains.

The electron affinity (EA) is the difference in energy between the lowest unoccupied molecular orbital and infinity for the grain of charge (Z - 1)e created by adding the electron (Weingartner and Draine (2001b)). EA is used in the calculation of photode-tachment threshold energy, which is discussed in Section 2.3.5.

 $E_{min}$  is the energy above infinity where, when an electron exceeds this energy, the tunnelling probability becomes significant (Weingartner and Draine (2001b)).

#### 2.3.2 Photoemission threshold energy

The photoemission threshold energy  $hv_{pet}$  is the minimum energy for which an incident photon can initiate the photoelectric effect on a certain dust grain (Weingartner and Draine (2001b)). It depends on the work function W of the grain (which depends on the grain composition; for carbonaceous grains, W = 4.4 eV, whereas W = 8.0 eV for silicate grains), the grain charge Z, the grain size and the photon energy (hv). Here, to simplify the calculations, it is assumed that all dust grains are spherical in shape with radius a, although small PAHs are planar molecules in reality.

In terms of the valence ionisation potential and  $E_{min}$  defined in 2.3.1,  $hv_{pet}$  is calculated by

$$h\nu_{\text{pet}}(Z,a) = \begin{cases} \text{IP}_{V}(Z,a), & Z \ge -1, \\ \text{IP}_{V}(Z,a) + E_{\min}(Z,a), & Z < -1. \end{cases}$$
(2.9)

#### 2.3.3 Photoemission threshold

Figures 2.3 and 2.4 show the effects of grain charge on photoemission threshold energy for 2 sizes of PAH grains. Especially for small grains, lowering the grain charge allows photons with lower energy to initiate the photoelectric effect.

<sup>&</sup>lt;sup>1</sup>One can express *e* in cgs units as  $e = 4.8 \times 10^{-10}$  esu and *a* in cm.  $e^2/a$  can then be calculated in ergs, which can be converted into eV for ease of calculation.



FIGURE 2.3: Effects of grain charge on photoemission threshold energy for PAH with a = 5 Å



FIGURE 2.4: Effects of grain charge on photoemission threshold energy for PAH with a = 20 Å

#### 2.3.4 Photoelectric yield

The photoelectric yield y is the probability that an electron will be ejected following the absorption of a photon. Fundamentally, y is dependent on four factors: (1) the grain composition (carbonaceous or silicate), since the material of the grain determines the optical properties of the grain; (2) the energy of the photon (hv), which

largely determines whether the photon has more energy than the photoemission energy; (3) the grain charge Z (y increases with lower Z); (4) radius of the grain a (in general, Y decreases with higher a).

The resulting expression for the photoelectric yield is

$$y(h\nu, Z, a) = y_2(h\nu, Z, a) \min[y_0(\Theta)y_1(a, h\nu), 1].$$
(2.10)

The definitions of these parameters are given in Appendix A.

#### 2.3.5 Photoelectric ejection of attached electrons (photodetachment)

WD01b included a "photodetachment" term specifically for grains with Z < 0, in which attached electrons are ejected after the grain absorbs a photon. They calculate the photodetachment threshold energy as

$$h\nu_{pdt}(Z < 0) = EA(Z + 1, a) + E_{min}(Z, a).$$
 (2.11)

#### 2.3.6 Effects of grain charge on photoelectric yield

Fig 2.5 displays the effects of grain charge on photoelectric yield for the smallest PAH grain. The plot clearly shows that the photoelectric yield is highly dependent on the grain charge.



FIGURE 2.5: Effects of grain charge on photoelectric yield for PAH with a = 5 Å. The optical properties (dielectric functions) of PAH utilise the dielectric functions used in a previous paper by Weingartner and Draine in 2001 (Weingartner and Draine (2001a))

#### 2.3.7 Grain charge distributions

Since the photoemission depends on the grain charge, it is necessary to know the distribution of charge states for the grains. In statistical equilibrium,

$$f_Z(Z)J_{\rm pe}(Z) = f_Z(Z+1)J_{\rm e}(Z+1),$$
 (2.12)

where  $f_Z(Z)$  is the probability for the grain charge to be Ze,  $J_{pe}$  is the photoemission rate and  $J_e$  is the electron accretion rate. WD01b's model also includes a  $J_{ion}$  term on the left hand side, denoting the positive ion accretion rate (e.g. accretion of protons onto the grains), but it is neglected here because of the large proton mass relative to the electron. Also, it is assumed that the number density of electrons is far greater than that of protons ( $n_e \gg n_p$ ), meaning that the proton accretion rate is negligible compared to the electron accretion rate. By iteratively applying Equation 2.12 and normalising,  $f_Z$  can be found for all Z.

#### 2.3.8 Photoemission rate

The photoemission rate is given by

$$J_{\rm pe}(a,Z) = \pi a^2 \int_{\nu_{\rm pet}}^{\nu_{\rm max}} y(h\nu,a,Z) Q_{\rm abs}(\nu) \frac{cu_{\nu}}{h\nu} \, d\nu + \int_{\nu_{\rm pdt}}^{\nu_{\rm max}} \sigma_{\rm pdt}(\nu) \frac{cu_{\nu}}{h\nu} \, d\nu, \qquad (2.13)$$

where  $Q_{abs}$  is the absorption efficiency. The second term in the above equation is only present when Z < 0.

#### 2.3.9 Electron accretion rate

The electron accretion rate is given by

$$J_{\rm e}(Z) = n_{\rm e} s_{\rm e}(Z) \left(\frac{8k_{\rm B}T}{\pi m_{\rm e}}\right)^{1/2} \pi a^2 \,\tilde{J}(\tau_{\rm e},\xi_{\rm e}),\tag{2.14}$$

where  $n_e$  is the electron density,  $s_e$  is the sticking coefficient of electron, which is the probability that an electron will transfer its charge if it reaches the surface of a grain of charge Ze,  $m_e$  is the electron mass, and  $\tilde{J}$  is a function of  $\tau_e \equiv ak_BT/e^2$  and  $\xi_e \equiv -Z$ . Expressions for  $\tilde{J}$  can be found in Draine and Sutin (1987).

#### 2.3.10 Calculating the total PE heating rate

After calculating the charge distribution  $f_Z(Z)$  for grains with radius *a*, the gas heating rate per grain due to photoelectric emission can be calculated by

$$\Gamma'_{\rm pe}(a) = \sum_{Z} f_{Z}(Z) \left[ \Gamma'_{\rm pe,\nu}(Z,a) + \Gamma'_{\rm pd}(Z,a) \right].$$
(2.15)

The contribution from the photoemission of valence electrons is

$$\Gamma_{\rm pe,\nu}'(Z,a) = \pi a^2 \int_{\nu_{\rm pet}(a,Z)}^{\nu_{\rm max}} y(a,Z,\nu) Q_{\rm abs}(a,\nu) \frac{cu_{\nu}(\nu)}{h\nu} \int_{E_{\rm min}}^{E_{\rm max}} f_E(E) E \, dE \, d\nu, \quad (2.16)$$

where  $E_{\min} = 0$  when  $Z \ge 0$  and is given by Equation A.5 when Z < 0,  $E_{\max} = h\nu - h\nu_{\text{pet}} + E_{\min}$ , the photoelectron energy distribution  $f_E(E) = f_E^0(E)/y_2$ . When Z < 0, the contribution from photodetachment is given by

$$\Gamma'_{\rm pd}(a) = \int_{\nu_{\rm pdt}}^{\nu_{\rm max}} \sigma_{\rm pdt}(\nu) \frac{cu_{\nu}}{h\nu} (h\nu - h\nu_{\rm pdt} + E_{\rm min}) \, \mathrm{d}\nu.$$
(2.17)

The total photoelectric heating rate in erg  $s^{-1}$  per H, after summing up the contribution from all grain sizes and all grain compositions, is

$$\Gamma_{\rm pe} = \sum_{\rm comp} \int_{a_{\rm min}}^{a_{\rm max}} \Gamma_{\rm pe}'(a) \frac{\mathrm{d}n_{\rm gr}}{\mathrm{d}a}(a) \,\mathrm{d}a, \tag{2.18}$$

where  $dn_{gr}/da$  is the number density of the dust grains in size interval da,  $\sum_{comp}$  means to sum up grains of different compositions in the grain model.

#### 2.3.11 Weingartner and Draine (2001a) grain model

As evident in Equation 2.18, the PE heating rate depends heavily on the grain model used. I use the grain model described in Weingartner and Draine (2001a) with  $R_V = 3.1$  and the abundance of carbon atoms in dust grains per hydrogen atom  $b_C = 6 \times 10^{-5}$ , but with grain abundances decreased by a factor of 0.93, as recommended by Draine (2004). Figure 2.6 shows the grain size distribution in the Weingartner and Draine (2001a) grain model.

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FIGURE 2.6: WD01 grain size distribution (Weingartner and Draine (2001a)). n(a) in the figure is equivalent to  $dn_{gr}/da$ .

# 2.4 Interfacing the PE heating model with radiation fields with arbitrary colour and amplitude

#### 2.4.1 The Mathis et al. (1983) radiation field

Having implemented an algorithm to calculate PE heating using the Weingartner and Draine (2001b) model, it remains to create a flexible interface with ISRFs of arbitrary intensities and colours. As a basic reference to construct ISRFs with different colours, I used the ISRF of Mathis, Mezger, and Panagia (1983) (Mathis ISRF). This ISRF is the estimate of the local ISRF at the solar neighbourhood in the Milky Way (with a galactocentric radius of 8 kpc). The ISRF is defined as:

$$\nu u_{\nu} = \begin{cases} 0, & \lambda < 0.0912 \ \mu m, \\ 1.287 \times 10^{-9} \ \lambda_{\mu m}^{4.4172}, & 0.0912 \ \mu m < \lambda < 0.11 \ \mu m, \\ 6.825 \times 10^{-13} \ \lambda_{\mu m}, & 0.11 \ \mu m < \lambda < 0.134 \ \mu m, \\ 2.373 \times 10^{-14} \ \lambda_{\mu m}^{-0.6678}, & 0.134 \ \mu m < \lambda < 0.246 \ \mu m, \\ \frac{4\pi \nu}{c} \sum_{i=1}^{3} w_{i} B_{\nu} T_{i}, & \lambda > 0.246 \ \mu m, \end{cases}$$
(2.19)

where

$$B_{\nu} = \frac{2h\nu^3}{c^2} \frac{1}{\exp(\frac{h\nu}{k_{\rm B}T}) - 1}$$
(2.20)

is the spectral brightness of the blackbody radiation and the blackbody components are  $w_1 = 1 \times 10^{-14}$ ,  $T_1 = 7500$  K,  $w_2 = 1 \times 10^{-13}$ ,  $T_2 = 4000$  K,  $w_3 = 1 \times 10^{-14}$ ,  $T_3 = 3000$  K.  $\lambda_{\mu m}$  stands for the value of photon wavelength in  $\mu m$ . The radiation is cut off at the ionisation energy of H<sub>I</sub> (912 Å). Figure 2.7 shows the Mathis ISRF in the range 912 Å  $< \lambda < 20$   $\mu m$ .



FIGURE 2.7: The Mathis, Mezger, and Panagia (1983) ISRF. For intuition purposes this plot is plotted against wavelength rather than photon frequency. Most of the energy in this radiation field lies in the near infrared (0.8  $\mu$ m <  $\lambda$  < 2.5  $\mu$ m).

The total energy density in the ISRF in the 6–13.6 eV interval is  $6.08 \times 10^{-14}$  erg cm<sup>-3</sup>, or  $G_0 = 1.14$ .

#### 2.4.2 Standard calculations with the Mathis ISRF

As a first test, I apply the PE heating model using the Mathis ISRF. Effects of the optical depth can be applied to the Mathis ISRF to simulate the attenuation of the ISRF in the presence of interstellar dust grains. Dust grains scatter and absorb photons in the ISRF and the overall process is called extinction. Since the absorption coefficient of dust grains increases with increasing frequency within the optical/FUV range, the absorption of photons by dust grains has the overall effect of reddening the ISRF.

The optical depth is related to the extinction cross-section of dust grains and the column density of hydrogen nuclei in the following way:

$$\tau(\nu) = C_{\text{ext}}(\nu) \cdot N_{\text{H}}, \qquad (2.21)$$

where  $C_{\text{ext}}$  is the extinction cross-section of the dust grains per H (in cm<sup>2</sup>), and  $N_{\text{H}}$  is the column density of hydrogen nuclei in cm<sup>-2</sup>. In the following calculations and throughout this thesis, the B-band optical depth ( $\tau_{\text{B}}$ ) is chosen as the quantity to characterise the extinction of the ISRF. This was done by normalising  $\tau(\nu)$  such that  $\tau(4451 \text{ Å}) = 1$  in the Weingartner and Draine (2001a) grain model. Here, 4451 Å is chosen as the representative wavelength of the B-band. It was found that

$$\tau_{\rm B} \equiv \tau(4451~{\rm \AA}) = 0.627~\left(\frac{N_{\rm H}}{1\times 10^{21}~{\rm cm}^{-2}}\right) \eqno(2.22)$$

for conditions of the solar neighbourhood (i.e.) with metallicity (relative to the solar value) unity, and the fraction of metals in grains as determined by Weingartner and Draine (2001a). This method quantifies the extinction with a connection more closely to the actual intensity of the ISRF. Figure 2.8 shows  $\tau(\nu)$  versus photon wavelength when  $\tau(4451 \text{ Å})$  is normalised to 1.



FIGURE 2.8:  $\tau(\nu)$  versus photon wavelength when  $\tau_B \equiv \tau(4451~\text{\AA})$  is normalised to 1

After calculating  $\tau(\nu)$  for the wavelength range from 912 Å to 8192 Å, the new SEDs are calculated by multiplying the SED of the Mathis with a scaling factor  $G_{ini}$  and the exponential of negative optical depth:

$$u'_{\nu}(\nu) = G_{\text{ini}} \cdot e^{-\tau(\nu)} \cdot u^{\text{Mathis}}_{\nu}(\nu), \qquad (2.23)$$

where  $u_{\nu}^{\text{Mathis}}$  is the SED of the Mathis ISRF. Figure 2.9 shows the extinction of the Mathis ISRF under different values of  $\tau_{\text{B}}$ .

2.4. Interfacing the PE heating model with radiation fields with arbitrary colour and amplitude



FIGURE 2.9: The extinction of Mathis et al. (1983) ISRF under different values of  $\tau_{\rm B}$ 

#### 2.4.3 Dividing the ISRF into 3 bands

To investigate the relative importance of UV/optical photons in PE heating, the radiation field is first divided into 3 bands: FUV, NUV and optical. The FUV band goes from 912 Å to 2089 Å, the NUV band goes from 2089 Å to 4169 Å and the optical band goes from 4169 Å to 8318 Å. Notice that the naming of these bands do not coincide with the usual usage of these bands. For example, the NUV extends to 4169 Å, even though electromagnetic radiation is already visible at  $\approx$ 3800 Å. The definition of the FUV band is similar to the conventional definition of FUV photons: 6 eV – 13.6 eV, and the rest of the spectrum (2089 Å to 8318 Å) is roughly divided in half logarithmically. Further details regarding the bands are given in Section 2.5.1.

To normalise the total intensity in each band with the Mathis ISRF, I define  $G_{FUV} \equiv \int u_{\nu} d\nu / u_{FUV}^{Mathis}$ , where the integration is between the limits of the FUV band and  $u_{FUV}^{Mathis}$  is the integrated energy density of the Mathis ISRF in the FUV band.  $G_{NUV}$  and  $G_{opt}$  are defined in a similar way. Again, further details are given in Section 2.5.1.

#### 2.4.4 The effects of optical depth on the Mathis ISRF

Figure 2.10 shows the attenuation of individual bands of the Mathis ISRF as a function of  $\tau_{\rm B}$  at T = 100 K and  $n_{\rm e} = 0.03$  cm<sup>-3</sup> (the typical conditions in the cold neutral medium). As the optical depth becomes higher, the reddening effect by the dust grains become more significant.



FIGURE 2.10: Intensity of Mathis ISRF under extinction

Figure 2.11 shows the components of PE heating rate due to the 3 bands in the Mathis ISRF. At  $\tau_{\rm B} < 3$ , FUV photons are the major contributors to PE heating. From  $\tau_{\rm B} = 3$  onwards, heating from optical photons starts to take over the heating from FUV photons. This shows that at high optical depths, considering only the FUV photons will lead to a severe underestimate of the true PE heating rate. Optical photons have to be considered in order to calculate the PE heating rate accurately.



FIGURE 2.11: Contribution to photoelectric heating from different bands in the Mathis ISRF

Figure 2.12 shows the comparison of the PE heating rate using the WD01b model ("full calculation") and the Bakes and Tielens (1994) model. Since it only takes the heating by FUV photons into account, the Bakes and Tielens (1994) model underestimates the PE heating rate by a factor of 2 at  $\tau_B = 3$ , and by orders of magnitude at high optical depth.



FIGURE 2.12: Comparing the photoelectric heating rate with Bakes & Tielens (1994) model

# 2.5 The photoelectric heating lookup table

As it is inefficient to calculate the photoelectric heating rate by solving for the grain charge distribution every time, a lookup table was designed so that the photoelectric heating rate can be calculated directly from the intensity and 'colour' of the radiation field, the electron density and gas temperature.

#### 2.5.1 Dividing the radiation field into 3 bands

The radiation field  $u_{\nu}$  is first divided into three bands: FUV, NUV, opt (optical). The bands are integrated with respect to frequency to obtain the corresponding G-factors

with respect to the Mathis field:

$$G_{\rm FUV} \equiv \frac{\int_{\nu_3}^{\nu_4} u_\nu(\nu) \,\mathrm{d}\nu}{u_{\rm FUV}^{\rm Mathis}},\tag{2.24}$$

$$G_{\rm NUV} \equiv \frac{\int_{\nu_2}^{\nu_3} u_{\nu}(\nu) \, \mathrm{d}\nu}{u_{\rm NUV}^{\rm Mathis}},\tag{2.25}$$

$$G_{\rm opt} \equiv \frac{\int_{\nu_1}^{\nu_2} u_{\nu}(\nu) \,\mathrm{d}\nu}{u_{\rm opt}^{\rm Mathis}},\tag{2.26}$$

where  $u_{FUV}^{\text{Mathis}}$  refers to the total energy density of the Mathis ISRF in the FUV band, with similar definitions for  $u_{\text{NUV}}^{\text{Mathis}}$  and  $u_{\text{opt}}^{\text{Mathis}}$ .

- 1/

| Table 2.1 displays the definitions | of the frequency constants | (boundary frequencies): |
|------------------------------------|----------------------------|-------------------------|
| 1 2                                | 1 2                        |                         |

| Constant       | Frequency (Hz)         | Corresponding wavelength (Å) | Corresponding energy (eV) |
|----------------|------------------------|------------------------------|---------------------------|
| $ u_4 $        | $3.2872\times10^{15}$  | 912                          | 13.60                     |
| ν <sub>3</sub> | $1.4351\times 10^{15}$ | 2089                         | 5.94                      |
| $\nu_2$        | $7.1910\times10^{14}$  | 4169                         | 2.97                      |
| $\nu_1$        | $3.6041\times 10^{14}$ | 8318                         | 1.49                      |

TABLE 2.1: Definition of the boundary frequencies

Integrating the SED of the Mathis ISRF gives the following constants:

$$u_{\rm FUV}^{\rm Mathis} \equiv 6.0837 \times 10^{-14} \,{\rm erg} \,{\rm cm}^{-3}$$
, (2.27)

$$u_{\rm NUV}^{\rm Mathis} \equiv 7.7613 \times 10^{-14} \, {\rm erg} \, {\rm cm}^{-3},$$
 (2.28)

$$u_{\rm opt}^{\rm Mathis} \equiv 2.0964 \times 10^{-13} \, {\rm erg} \, {\rm cm}^{-3}.$$
 (2.29)

Since the FUV band determines the overall heating and grain charging in most cases, the FUV is further divided into two sub-bands: a short-wavelength sub-band and a long-wavelength sub-band. The boundary between the sub-bands is chosen as the mid-point between  $v_3$  and  $v_4$  in logarithmic space:

$$\nu_{\rm m} = 2.1720 \times 10^{15} \,{\rm Hz} \,\,(1380 \,{\rm \AA}/8.98 \,{\rm eV}).$$
 (2.30)

The "colour" of the FUV band is defined as the ratio between the energy densities of the two sub-bands, or

$$\operatorname{col}_{\mathrm{FUV}} = \frac{\int_{\nu_{\mathrm{m}}}^{\nu_{4}} u_{\nu}(\nu) \, \mathrm{d}\nu}{\int_{\nu_{3}}^{\nu_{\mathrm{m}}} u_{\nu}(\nu) \, \mathrm{d}\nu}.$$
(2.31)

The FUV colour of the Mathis field is 0.8862.

Figure 2.13 shows the Mathis ISRF with the boundary frequencies and  $\nu_{\rm m}$  indicated.



FIGURE 2.13: SED of the Mathis ISRF with the boundary wavelengths labelled

#### 2.5.2 Creating new SEDs from the Mathis ISRF

SEDs with different relative strengths in the FUV, NUV and optical bands are created from the Mathis ISRF by the following way:

1. Take the mid-band frequencies of the FUV, NUV and optical bands (in logarithmic scale); I call them  $\nu_{FUV}$ ,  $\nu_{NUV}$  and  $\nu_{opt}$  (incidentally,  $\nu_{FUV} = \nu_m$ ). These mid-band frequencies are shown as dotted lines in Figure 2.14 and their definitions are shown in Table 2.2.

| Constant         | Frequency (Hz)        | Corresponding wavelength (Å) |
|------------------|-----------------------|------------------------------|
| $ u_{\rm FUV}$   | $2.1720\times10^{15}$ | 1380                         |
| $\nu_{ m NUV}$   | $1.0159\times10^{15}$ | 2952                         |
| V <sub>opt</sub> | $5.0909\times10^{14}$ | 5889                         |

TABLE 2.2: Definition of the mid-band frequencies

2. Define a 3-element vector  $\vec{W} = (W_{FUV}, W_{NUV}, W_{opt})$ .  $W_{FUV}, W_{NUV}$  and  $W_{opt}$  are used to scale up/down the Mathis ISRF at the mid-band frequencies according

to  $u_{\nu}^{\text{new}}(\nu_{\text{FUV}}) = 10^{W_{\text{FUV}}} \cdot u_{\nu}(\nu_{\text{FUV}})$  for the FUV band, and similarly for NUV and opt bands. I define a general element in  $\vec{W}$  as W. W can take one of the 15 values in the following list:

$$W \in (-3.0, -2.5, -2.0, -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0)$$
(2.32)

3. For each *W*, choose a number from the list above. Then construct a function W(v) by joining the *W*s with straight lines in logarithmic space and extrapolate if necessary. Mathematically, W(v) is defined as:

$$W(\nu) = \begin{cases} \frac{W_{\text{NUV}} - W_{\text{opt}}}{\log \nu_{\text{NUV}} - \log \nu_{\text{opt}}} (\log \nu - \log \nu_{\text{opt}}) + W_{\text{opt}}, & \text{for } \nu_1 \le \nu < \nu_{\text{NUV}}, \\ \frac{W_{\text{FUV}} - W_{\text{NUV}}}{\log \nu_{\text{FUV}} - \log \nu_{\text{NUV}}} (\log \nu - \log \nu_{\text{NUV}}) + W_{\text{NUV}}, & \text{for } \nu_{\text{NUV}} \le \nu \le \nu_4. \end{cases}$$

$$(2.33)$$

As an example, Figure 2.14 shows the construction of  $W(\nu)$  from  $\vec{W} = (0, 2, 1)$ .



FIGURE 2.14: The construction of  $W(\nu)$  from  $\vec{W} = (0, 2, 1)$ 

4. Form a new SED by multiplying the SED of the Mathis ISRF with  $10^{W(\nu)}$ :

$$u_{\nu}^{\text{new}}(\nu) = u_{\nu}^{\text{Mathis}}(\nu) \cdot 10^{W(\nu)}.$$
(2.34)

5. The W values are iterated over the W-list (Equation 2.32), so  $15^3 = 3375$  SEDs are created. In ascending order of frequency, the new SEDs in each band are

combined to form a new SED. The new SED is integrated in each band to obtain  $\vec{G} \equiv (G_{\text{FUV}}, G_{\text{NUV}}, G_{\text{opt}})$ . For example, if  $\vec{W} = (0, 2, 1)$  (as in the example above),  $\vec{G} = (G_{\text{FUV}}, G_{\text{NUV}}, G_{\text{opt}}) = (2.465, 52.41, 10.71)$ .



FIGURE 2.15: Creating a new ISRF from  $W(\nu)$  and the Mathis ISRF

Then the full calculation of PE heating rate (per hydrogen) is performed using this new SED, T = 100 K and a certain value of  $n_e$ .  $n_e$  (in cm<sup>-3</sup>) is chosen from one of the values from this list:  $\{3 \times 10^{-4}, 3 \times 10^{-3}, 3 \times 10^{-2}, 3 \times 10^{-1}, 3 \times 10^{0}\}$ . So, in total, including the sampling for  $n_e$ , the lookup table contains  $5 \times 15^3 = 16875$  elements. The dimensions of the PE lookup table is 5\*15\*15\*15.

#### 2.5.3 Construction of the lookup table

Given a certain input SED, in principle, within the space of  $\vec{W}$ , there should be a vector value of  $\vec{W}$  (call it  $\vec{W}_{min}$ ) that generates an SED from the Mathis ISRF which is the most similar to that particular input SED. Since  $\vec{W}_{min}$  is difficult to find, it is easier to interpolate the PE heating in  $\vec{G}$ -space rather than in  $\vec{W}$ -space. Therefore, another lookup table was created for the interpolation of PE heating in  $\vec{G}$ -space. Six quantities (heat\_FUV, heat\_NUV, heat\_opt, G\_FUV, G\_NUV and G\_opt) are stored within one coordinate in the lookup table ([i\_n\_e, i\_W\_FUV, i\_W\_NUV, i\_W\_opt]). i\_n\_e is the index of the electron density and i\_W\_FUV is the index of  $W_{FUV}$ . heat\_FUV is the PE heating the SED with  $\vec{W} = (0,2,1)$ , if  $n_e = 3 \times 10^{-2}$  cm<sup>-3</sup>, the values  $G_{FUV} = 2.465$ ,  $G_{NUV} = 52.41$ ,  $G_{opt} = 10.71$ , together with heat\_FUV, heat\_NUV and heat\_opt, are stored in the coordinate [2,6,10,8].

#### 2.5.4 Interpolation of PE heating from the lookup table

To interpolate the PE heating rate from any SED, the G-factors must first be known. In BT94's analytic approximation of PE heating rate, grain charging depends on  $G_0\sqrt{T}/n_{\rm e}$ . To investigate the relationship between grain charging, the gas temperature and the electron density (without the influence of the ISRF), I first define  $\gamma' \equiv \sqrt{T}/n_{\rm e}$ . Since the radiation field is already accounted for by the lookup table, the table tabulates  $\gamma'$  with the following values (in K<sup>1/2</sup> cm<sup>3</sup>):

$$\gamma' \in (3.33 \times 10^4, 3.33 \times 10^3, 3.33 \times 10^2, 3.33 \times 10^1, 3.33).$$
 (2.35)

To interpolate the heating of an SED with certain values of *T* and  $n_e$ , a heating list of 5 elements is first created with the known  $G_{\text{FUV}}$ ,  $G_{\text{NUV}}$ ,  $G_{\text{opt}}$  values, interpolated between the grid in the lookup table and using the  $\gamma'$  values defined above. For example, to find the heating rate due to an SED with G-factors  $(10^{2.4}, 10^{1.7}, 10^{0.9})$ , T = 80K and  $n_e = 0.01 \text{ cm}^{-3}$ , the heating rates are interpolated within the grid with boundaries  $2.0 < W_{\text{FUV}} < 2.5, 1.5 < W_{\text{NUV}} < 2.0, 0.5 < W_{\text{opt}} < 1.0$ . Then, the true interpolated heating rate is obtained by interpolating again with  $\gamma' = \sqrt{80}/0.01 \text{ K}^{1/2} \text{ cm}^3$ among the  $\gamma'$ -list. Note that the interpolation between the *W*-grid and the interpolation among the  $\gamma'$ -list are both done in logarithmic space. For reasons discussed below, the total heating and the heating due to the FUV band are interpolated separately. Figure 2.16 shows how to interpolate the total PE heating rate with  $\gamma'$ .



FIGURE 2.16: Example of interpolating by  $\gamma' = \sqrt{T}/n_e$  in the Mathis ISRF

#### 2.5.5 FUV colour correction

The above interpolation process assumes that the input SED has the same in-band "colour" as the Mathis ISRF, which is not always the case. This is particularly important in the FUV band, as is also evident in the example in Figure 2.14, where the radiation is redder than the Mathis ISRF template within the band. Therefore, it is necessary to correct for the in-band colours. Since the FUV band determines the overall heating and grain charging in most cases, only the colour of the FUV band is corrected. If the FUV colour is "bluer" than the Mathis ISRF (col\_FUV > col\_FUV\_Mathis), the FUV heating will be underestimated. On the other hand, an SED with a very red FUV spectrum will lead to an overestimation of its FUV heating rate.

The method is to first generate some SEDs with different colours to the Mathis ISRF, calculate their PE heating rate arising from the FUV band (the actual FUV heating, heat\_FUV\_act) and the FUV heating interpolated from the lookup table (heat\_FUV\_LUT).heat\_FUV\_ratio is calculated to be the ratio of heat\_FUV\_LUT to heat\_FUV\_act:

$$heat_FUV_ratio = \frac{heat_FUV_LUT}{heat_FUV_act}.$$
 (2.36)

It was found that for SEDs with similar  $G_{FUV}$  values, their heat\_FUV\_ratio is well correlated to their FUV colours. Figure 2.17 demonstrates the correlation between heat\_FUV\_ratio and the FUV colour for  $-2.0 < \log(G_{FUV}) < -1.5$ .



FIGURE 2.17: Correlation between heat\_FUV\_ratio and the FUV colour for  $-2.0 < \log(G_{FUV}) < -1.5$ 

Therefore, it is possible to correct for the effects of FUV colours to have a more accurate estimation of the PE heating rate:

$$heat_without_FUV = heat_LUT - heat_FUV_LUT,$$
 (2.37)

$$heat = \frac{heat_FUV_LUT}{heat_FUV_ratio} + heat_without_FUV.$$
(2.38)

where heat is the final interpolated total PE heating rate.

# **2.5.6** Extrapolation of PE heating rate beyond the boundaries of *G*<sub>FUV</sub> in the lookup table

If log  $G_{FUV} > 4.0$ , the PE heating rate is extrapolated from the heating rate at log  $G_{FUV} = 3.5$  and log  $G_{FUV} = 4.0$ . If log  $G_{FUV} < -3.0$ , the PE heating rate is extrapolated from the heating rate at log  $G_{FUV} = -2.5$  and log  $G_{FUV} = -3.0$ .

#### 2.5.7 Usage

To use the PE lookup table, the user has to input six quantities to the program:  $G_{FUV}$ ,  $G_{NUV}$ ,  $G_{opt}$ ,  $col_{FUV}$ , T and  $n_e$ . The program will output a single value for the estimated PE heating rate per H, in erg s<sup>-1</sup> H<sup>-1</sup>.

#### 2.5.8 Effectiveness of the lookup table

To test the effectiveness of the PE lookup table, 900 SEDs are simulated by varying the colours of individual bands of the Mathis ISRF and changing the integrated energy density in each band. The PE heating rates of 889 SEDs has suitable  $G_{FUV}$ values and their actual and interpolated heating rates are calculated. Figures 2.18 and 2.19 show the percentage error in the predicted heating of these SEDs (error = (heat\_predicted-heat\_actual)/heat\_actual). Figure 2.19 is a zoom-in of Figure 2.18 in the range -110% to +150%.



FIGURE 2.18: Percentage error in the predicted PE heating of 889 simulated SEDs before and after FUV colour correction



FIGURE 2.19: Same as Figure 2.18, but zooms into the region -110% to +150%

The error in heating prediction is greatly reduced after the effects of the FUV colour have been corrected. After colour correction, the error in heating prediction from 75% SEDs are within 20% of the actual values. This is sufficient for fast calculations in iterative schemes to solve for the balance between gas heating and cooling. Near the solution, a switch can be made to the accurate solution using the full calculation.

Figure 2.20 shows a good fit between the full model and the PE database method in calculating the PE heating rate of the attenuated Mathis ISRF. As  $\tau_{\rm B}$  increases, the value of  $G_{\rm FUV}$  decreases (going from right to left on the x-axis). There is only a significant discrepancy between the values calculated by the database and the full model when the radiation field is very red and very weak in the FUV band.



FIGURE 2.20: Comparison of full calculation versus PE heating database for low  $G_{FUV}$  values, using 2.23 to attenuate the Mathis ISRF

Figure 2.21 shows a similarly good fit for an unattenuated radiation field that is very strong in FUV ( $G_{ini} = 10^4$ ). There is very good fit for  $G_{FUV} \le 3 \times 10^3$ .



FIGURE 2.21: Comparison of full calculation versus PE heating database for high  $G_{FUV}$  values, using 2.23 to attenuate an ISRF with  $G_{ini} = 10^4$  and the shape of Mathis ISRF

The full PE heating model provides the backbone of the self-consistent ISM thermodynamic model, which incorporates an originally formulated chemical model. This is the topic of Chapter 3. The following section explores the effects of the radiation field on the grain charge distribution.

# 2.6 Grain charge distributions

This section explores the effects of grain composition, radiation field and electron density on the charge distributions of grain charges.

#### 2.6.1 The effects of grain composition

Figure 2.22 shows the grain charge distribution of PAH and silicate grains in Mathis ISRF, both with radius 10 Å. Due to the higher work function of silicate grains, fewer photons can initiate the photoelectric effect on them, so they have lower grain charge than PAH grains.



FIGURE 2.22: Grain charge distributions of 10 Å PAH and silicate grains, in Mathis ISRF, T = 100 K,  $n_e = 0.02$  cm<sup>-3</sup>

#### 2.6.2 The effects of radiation field

In Figure 2.23, the Mathis ISRF is scaled with  $G_{ini}$  while  $\tau_B$  is kept as 0. On average, the PAH grains are more positively charged in stronger radiation fields. Bigger grains have a wider range of charge states that are physically possible (Weingartner and Draine (2001b)) and this effect is more apparent in strong radiation fields.



FIGURE 2.23: Grain charge distributions for three sizes of PAH grains, under 3 intensities of ISRF. T = 100 K
# 2.6.3 The effects of optical depth

In Figure 2.24, the Mathis ISRF is attenuated by the optical depth function  $\tau(\nu)$ , and  $G_{\text{ini}} = 1$ . As  $\tau_{\text{B}}$  increases, the grains become more negatively charged. Increasing  $\tau_{\text{B}}$  also has the effect of narrowing the grain charge distribution of big grains.



FIGURE 2.24: Effects of ISRF colours on the grain charge distributions of PAH grains. T = 100 K.

#### 2.6.4 The effects of electron density

In Figure 2.25, three different electron density values are applied to the PE heating model with Mathis ISRF. The grains become significantly more negatively charged when  $n_e$  is increased.



FIGURE 2.25: Effects of electron density on the grain charge distributions of PAH grains. Mathis ISRF, T = 100 K.

# 2.7 Variation of PE heating efficiency with grain charging

The following plots show  $\epsilon$  versus  $G_{ini}\sqrt{T}/n_e$ , where  $\epsilon$ , the PE heating efficiency, is defined as

$$\epsilon \equiv \frac{\Gamma_{\rm PE}}{G_{\rm FUV} \cdot 10^{-24} \,\rm erg \, s^{-1}} \tag{2.39}$$

where  $\Gamma_{\text{PE}}$  is the PE heating rate per H. The definition of  $\epsilon$  is inspired by the PE heating efficiency parameter in Bakes and Tielens (1994), in which  $\epsilon$  is also used as the symbol for this quantity.



FIGURE 2.26: Comparison of PE heating efficiency for BT94 model and YFW model (the model described in this thesis). Here  $\tau_{\rm B} = 0$ .



FIGURE 2.27: Effects of optical depth on PE heating efficiency

In Figures 2.28-2.36, the Mathis ISRF is scaled and attenuated according to Eq.2.23. The PE heating per H from FUV, NUV and optical bands are calculated individually. The effects of intensity and colour of the ISRF and PE heating rate are investigated

under the circumstances that the  $\sqrt{T}/n_e$  is constant. Comparing a cold diffuse cloud with a molecular cloud, *T* may span an order of magnitude but  $n_e$  may span for 3 orders of magnitude or more. Therefore,  $n_e$  usually has a much bigger impact on the value of  $\sqrt{T}/n_e$  than *T*, hence it affects the grain charging more.

# 2.8 Variation of PE heating rate with radiation field

This section investigates the variation of PE heating rate in radiation fields with different intensities and colours. The investigation is done in 3 values of  $\gamma' = \sqrt{T}/n_e$ :

- 1.  $\gamma' = 500 \text{ K}^{1/2} \text{ cm}^3$  (*T* = 100 K and  $n_e = 0.02 \text{ cm}^{-3}$ )
- 2.  $\gamma' = 5 \times 10^3 \text{ K}^{1/2} \text{ cm}^3$  (*T* = 100 K and  $n_e = 2 \times 10^{-3} \text{ cm}^{-3}$ )

3. 
$$\gamma' = 50 \text{ K}^{1/2} \text{ cm}^3$$
 ( $T = 100 \text{ K}$  and  $n_e = 0.2 \text{ cm}^{-3}$ )

The contribution to PE heating by NUV and optical photons is also investigated.

# **2.8.1** $\gamma' = 500 \text{ K}^{1/2} \text{ cm}^3$

In the following figures, T = 100 K and  $n_e = 0.02$  cm<sup>-3</sup> ( $\gamma' = 500$  K<sup>1/2</sup> cm<sup>3</sup>). These values are typical in the cold neutral medium in the solar neighbourhood.



FIGURE 2.28: For  $\gamma' = 500 \text{ K}^{1/2} \text{ cm}^3$ . The contour lines show log  $\Gamma_{\text{PE}}$ , where  $\Gamma_{\text{PE}}$  is the total PE heating per H in erg s<sup>-1</sup> H<sup>-1</sup>.

In Figure 2.28, the PE heating per H decreases with decreasing  $G_{ini}$  and/or increasing  $\tau_B$ . Figure 2.29 shows the fraction of PE heating coming from NUV and optical photons. When  $G_{ini}$  is low and  $\tau_B$  is high, NUV and optical photons can produce more than 99% of the total PE heating.



FIGURE 2.29: Fraction of PE heating from NUV and optical photons for  $\gamma' = 500 \text{ K}^{1/2} \text{ cm}^3$ 

Figure 2.30 shows the fraction of PE heating coming from optical photons. When  $G_{ini}$  is low and  $\tau_B$  is high, optical photons produce more than 95% of the total PE heating.



FIGURE 2.30: Fraction of PE heating from optical photons for  $\gamma'=500~{\rm K}^{1/2}~{\rm cm}^3$ 

# **2.8.2** $\gamma' = 5 \times 10^3 \text{ K}^{1/2} \text{ cm}^3$

As expected, the PE heating rate is lower due to the grains being more positively charged, and this is most evident at high  $G_{ini}$  (Figure 2.31). However, the fraction of heating from NUV and optical photons can still exceed 95% if the radiation field is very red (Figure 2.32).



FIGURE 2.31: PE heating rate for  $\gamma'=5\times 10^3~K^{1/2}~cm^3$ 



FIGURE 2.32: Fraction of PE heating by NUV and optical photons for  $\gamma'=5\times 10^3~{\rm K}^{1/2}~{\rm cm}^3$ 



FIGURE 2.33: Fraction of PE heating by optical photons for  $\gamma'=5\times10^3~K^{1/2}~cm^3$ 

# **2.8.3** $\gamma' = 50 \text{ K}^{1/2} \text{ cm}^3$

The PE heating rate is higher due to the grains being more negatively charged. The shape of the contour lines is similar to high  $\gamma'$  values.



FIGURE 2.34: PE heating rate for  $\gamma' = 50 \text{ K}^{1/2} \text{ cm}^3$ 



FIGURE 2.35: Fraction of PE heating by NUV and optical photons for  $\gamma'=50~{\rm K}^{1/2}~{\rm cm}^3$ 

As Figure 2.36 shows, optical photons alone can produce the vast majority of PE heating if  $\gamma'$  is low and the radiation field is very "red". This can happen if the ionisation fraction is high while the FUV intensity is low: for example, in molecular cloud cores with high CR flux. This effect will be demonstrated in Section 3.12 in the next chapter.



FIGURE 2.36: Fraction of PE heating by optical photons for  $\gamma'=50\,{\rm K}^{1/2}\,{\rm cm}^3$ 

From these plots, it can be concluded that the PE heating from NUV and optical photons can become important in highly obscured regions in the interstellar medium, where the colour of the radiation field is very "red". This is especially the case if the grain charging parameter is low, which can happen in regions in galaxies with high CR flux (and low gas temperature) and/or in regions in galaxies with a high absolute level of optical light illuminating clouds, such as in the central regions of galaxies.

# **Chapter 3**

# A simple model of chemistry in the neutral and molecular ISM

# 3.1 Introduction

As discussed in Chapter 2, PE heating is an important heating component of the neutral and molecular ISM, affecting the thermodynamic state of the gas. In Chapter 2 I described an extension of an existing model of PE heating that accounts for the colour, as well as the intensity of the radiation field. To see the effects of PE heating, and to judge its relative importance to other heating components, such as CR heating, I need to incorporate the new PE heating model in a basic model for the heating and cooling of the ISM. This model also forms the basis for large-scale radiative transfer calculation of clouds in the ISM in galaxies (Chapter 5). To this end one needs to solve for:

- 1. chemistry
- 2. radiative transfer (RT)
- 3. physical properties of self-gravitating clouds

In this chapter, I consider the chemistry. I adopt existing models, but with the prime variable external pressure  $P_{\text{ext}}$  (rather than the gas density *n* or hydrogen nuclei density  $n_{\text{H}}$ ) as it is more suitable for interfacing with models of self-gravitating clouds. In addition, in contrast to existing models, I strictly separate the the portion of the chemistry problem from the RT problem. That is, I only consider the external pressure  $P_{\text{ext}}$ , the *in situ* ISRF (of course with colour), and *in situ* CRs as the model inputs. In this chapter, I will consider the thermal pressure  $P_{\text{therm}}$  comprising the totality of the pressure of a cloud, and explore model predictions for the effects of cosmic rays on gas heating and chemistry. In Chapter 4, other pressure terms are incorporated into the model.

#### 3.1.1 A short note on notation

Throughout this thesis, I use the spectroscopic notation (e.g. (C II)) and the chemical notation (e.g.  $(C^+)$ ) interchangeably. The spectroscopic notation is used when the

topic is line emission, whereas the chemical notation is used in chemical reactions. This may lead to some confusion, but I believe the chemical notation is more suitable when discussing chemistry-related topics.

# 3.2 Inputs to the model

1. Interstellar radiation field

The interstellar radiation field (ISRF) is arguably the most important input of the model, as the majority of the energy input into interstellar clouds comes from it, except in the case where the CR ionisation rate is very high and the ISRF is very weak. The model accepts two forms for the input ISRF:

- (a) as an SED  $(u_{\nu}(\nu))$  in the form of a 17-element vector within a frequency grid. The minimum frequency  $\nu_{\min}$  (=  $\nu_1$ ) is 3.604 × 10<sup>14</sup> Hz, corresponding to  $\lambda = 8318$  Å. The Lyman limit ( $\lambda = 912$  Å) is taken to be the maximum frequency  $\nu_{\max}$  (=  $\nu_4$ ), which is equal to  $3.287 \times 10^{15}$  Hz. 15 additional frequencies are divided between  $\nu_{\min}$  and  $\nu_{\max}$ , with equal intervals in logarithmic space. Figure 3.1 shows the frequency grid with the Mathis ISRF for reference.
- (b) in the form of a three-element vector parameter  $G_{vtr}$  and a scalar parameter  $col_{FUV}$ . The model calculates a  $u_v$  with 4 frequency values internally for calculating the radiative heating of dust grains. The PE heating is estimated with the inputs  $G_{vtr}$  and  $col_{FUV}$  using the PE lookup table described in Section 2.5.



FIGURE 3.1: The 17-element frequency list for the input  $u_v$ . The Mathis ISRF is plotted in the background for reference. For ease of understanding, the x-axis is in wavelength rather than in frequency. Also shown are the boundary frequencies and  $v_m$  defined in Chapter 2.

2. Thermal pressure ( $P_{\text{therm}}$ )

Thermal pressure is a major component of pressure in the cold neutral medium. In this chapter, it is assumed that the pressure of the gas is fully supported by the thermal pressure. In Chapter 4 the other pressure terms, such as CR pressure and magnetic pressure, are incorporated into the total pressure. The units of  $P_{\text{therm}}$  are  $k_{\text{B}}$  K cm<sup>-3</sup>.

3. Primary cosmic ray ionisation rate of hydrogen ( $\zeta_p$ ), in s<sup>-1</sup>

As mentioned in Section 1.5, cosmic ray ionisation is source of gas heating and free electrons in the neutral and molecular ISM. The primary cosmic ray ionisation rate (CRIR) per hydrogen atom (H I),  $\zeta_p$ , is chosen to be the fundamental parameter, as opposed to the total CRIR per hydrogen atom ( $\zeta_{HI}$ ) or the total CRIR per H<sub>2</sub> ( $\zeta_{H_2}$ ), since  $\zeta_p$  relates to the total flux of CR irradiating the gas.  $\zeta_{HI}$  and  $\zeta_{H_2}$  include the primary ionisations of hydrogen by cosmic rays, as well as the secondary ionisation by the energetic (secondary) electrons produced in the primary ionisation event. Under the typical conditions of the diffuse neutral ISM, the rough relationship between the 3 rates is given by  $\zeta_p = \zeta_{HI}/1.5 = \zeta_{H_2}/2.3$  (Glassgold and Langer (1974)). My analysis takes into account the dependence of total ionisation rate on the molecular fraction.

#### 4. Metallicity (Z') (unitless)

The metallicity constrains the total abundance of metals in the gas and the dust. In the model, the metallicity is parametrised relative to the solar metallicity ( $Z' = Z_{metal}/Z_{\odot}$ , where  $Z_{metal}$  is the absolute value of metallicity and  $Z_{\odot}$  is the solar metallicity). To be consistent with the Weingartner and Draine (2001a) (WD01a) dust model I am using, I use the same solar metallicity values for carbon and oxygen as they did (Grevesse and Sauval (1998)). In the model, the solar metallicity and helium abundance have the following values:  $x_{\text{He},\odot} = 8.511 \times 10^{-2}$  – fractional abundance of helium (by number) in the Sun, relative to hydrogen (Asplund et al. (2009)),  $x_{\text{C},\odot} = 3.31 \times 10^{-4}$  – fractional abundance of carbon (by number) in the Sun, relative to hydrogen (Grevesse and Sauval (1998)),  $x_{\text{O},\odot} = 6.76 \times 10^{-4}$  – fractional abundance of oxygen (by number) in the Sun, relative to hydrogen (Grevesse and Sauval (1998)).

5. Fraction of metals in grains  $(F_{gr})$  (unitless)

This quantity constrains the total number of atoms of a specific element in the dust. It is the fraction of atoms (of a specific element) that is present in dust grains, out of the totality of gas and dust in the ISM.  $1 - F_{gr}$  is therefore the depletion of metal in the interstellar gas (see the review by Savage and Sembach (1996), where the depletion of element *X* is denoted by  $\delta(X)$ ). This quantity may be different for carbon and for oxygen, so  $F_{gr}$  is represented by a 2-element vector:  $F_{gr} = [F_{gr,C}, F_{gr,O}]$ . The fraction of carbon atoms in grains (relative to hydrogen) is defined as  $x_{C,gr} \equiv n_{C,gr}/n_{H}$ . A corresponding quantity can be defined for oxygen (denoted as  $x_{O,gr}$ ).

The fraction of carbon atoms in grains is defined as

$$F_{\rm gr,C} \equiv \frac{x_{\rm C,gr}}{Z' x_{\rm C,\odot}}.$$
(3.1)

The abundance C atoms in the gas phase relative to hydrogen  $(x_{C,g})$  can be expressed as

$$\begin{aligned} x_{\mathsf{C},\mathsf{g}} &= x_{\mathsf{C},\mathsf{tot}} - x_{\mathsf{C},\mathsf{gr}} \\ &= Z' x_{\mathsf{C},\odot} - F_{\mathsf{gr},\mathsf{C}} x_{\mathsf{C}} \\ &= (1 - F_{\mathsf{gr},\mathsf{C}}) Z' x_{\mathsf{C},\odot}. \end{aligned}$$

The total number density of C atoms in the gas phase is then equal to  $n_{C,g} =$ 

 $x_{C,g}n_{H}$ .  $x_{O,g}$  can be obtained in a similar way.  $F_{gr}$  is an important factor defining a dust model. Following the assumed depletion ratios in WD01a, the default values of both  $F_{gr,C}$  and  $F_{gr,O}$  that I use here are 0.7. Unless otherwise stated, these values are used in the calculations in this thesis.

This model does not model the freeze-out of molecules onto dust grains at very low gas temperatures (see Section 3.3) or the process of grain sputtering in hot gas. In addition, it is assumed that there are no grain-surface reactions except the formation of  $H_2$ , as these reactions are limited in the diffuse phases of the ISM due to the effects of photodesorption (Tielens (2005)), so there is no exchange of atoms between the gas phase and the solid phase (the dust). The abundance of a certain element in the gas phase and the solid phase is constant in the model.

6. Intensity of the infrared/microwave background radiation field at the emission lines, in erg cm<sup>-2</sup> s<sup>-1</sup> Hz<sup>-1</sup>

To calculate the line emission of a given species, it is necessary to know the populations of energy levels, which are computed in the model and described in Section 3.10. These are influenced by the stimulated excitation and deexcitation induced by the infrared (IR)/microwave photons at the line frequencies. This model deliberately does not calculate the radiative transfer of the radiation field, so a IR/microwave background radiation field has to be supplied as an input to the model. Although it is possible to supply a custom background radiation field as an input, I performed the calculations in Chapters 3 and 4 in this thesis using the cosmic microwave background radiation field at the emission lines. This is the IR/microwave background radiation field used in the model by default. The CMB radiation very closely follows a blackbody radiation spectrum:

$$I_{\nu,\text{CMB}} = B_{\nu}(\nu, T_{\text{CMB}}) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(\frac{h\nu}{k_{\text{B}}T_{\text{CMB}}}) - 1'}$$
(3.2)

where  $T_{\text{CMB}} = 2.726$  K, as measured by the *COBE* FIRAS instrument (Mather et al. (1994)).

### **3.3** Outputs of the model

1. gas temperature (T), in K

The gas temperature is a gauge to the average kinetic energy of the atoms and molecules composing the interstellar gas. In this model, if the gas temperature drops below 8 K, the calculation is halted immediately as molecules tend to freeze out in the cold cores of molecular clouds at a gas temperature of around 10 K (Steinacker (2016)). As this model does not model the freezeout of molecules onto dust grains at very low temperatures, the model stops the calculation when the gas temperature falls below 8 K. For  $n_{\rm H} \sim 10^4$  cm<sup>-3</sup>, even if the dust temperature drops below 20 K, the freeze-out timescale will be  $\sim 10^6$  years (Williams and Viti (2013)) and could be safely neglected in my calculations.

2. number density of hydrogen nuclei ( $n_{\rm H}$ ), in cm<sup>-3</sup>

In this model,  $n_{\rm H}$  includes the hydrogen atoms in H<sub>I</sub> and H<sub>2</sub>:  $n_{\rm H} = n_{\rm H_I} + 2n_{\rm H_2}$ . In theory, it should also include hydrogen in other forms (e.g. H<sup>+</sup>, H<sup>+</sup><sub>2</sub>, H<sup>+</sup><sub>3</sub>), as they are present in the model. However, since this model only applies to the cold neutral and molecular medium, it can be assumed that the ionisation fraction is low enough ( $x_{\rm e} \ll 0.1$ ) that the number densities of the hydrogen cations are negligible compared to H and H<sub>2</sub>. It is also assumed that the metallicity is not so high, so that  $x_{\rm C,g} \ll 1$  and  $x_{\rm O,g} \ll 1$ .

3. molecular fraction  $(f_{H_2})$  (unitless)

The molecular fraction is a unitless value between 0 and 1. It is defined as

$$f_{\rm H_2} \equiv \frac{2n_{\rm H_2}}{n_{\rm H}}.$$
 (3.3)

If  $f_{H_2} = 0$ , the gas is fully atomic; if  $f_{H_2} = 1$ , the gas is fully molecular.  $f_{H_2}$  represents the proportion of hydrogen atoms in H<sub>I</sub> and H<sub>2</sub> that are in H<sub>2</sub> molecules. Similar to the definition of  $n_{H_1}$ , it neglects the hydrogen cations.

- 4. number densities of chemical species ( $n_X$ ), in cm<sup>-3</sup>
  - Including electrons, there are 12 chemical species in this model: H, H<sub>2</sub>, H<sup>+</sup>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, He, He<sup>+</sup>, C<sup>+</sup>, C, CO, O, and e<sup>-</sup>. The choice of the chemical species is to include the major species in the gas (H, H<sub>2</sub> and He), the ionisation products of these species by cosmic rays (H<sup>+</sup>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, and He<sup>+</sup>), and the species that produce observationally dominant lines (C<sup>+</sup>, C, CO and O). The final list of species are chosen to be those that dominate the cooling of the gas in the neutral and molecular ISM. The abundances of the chemical species relative to total hydrogen ( $x_X$ ) can be easily obtained by dividing  $n_X$  by  $n_{\rm H}$ .
- 5. gas heating and cooling rates ( $\Gamma_X$ ,  $\Lambda_X$ ), in erg s<sup>-1</sup> per hydrogen atom  $\Gamma_X$  refers to the gas heating rate per H due to process X and  $\Lambda_X$  refers to the gas cooling rate per H due to process X. Specifically, for the PE heating rate, the model outputs the heating rate due to FUV photons, NUV photons and optical photons individually.

6. line emissivities (j(X)), in erg cm<sup>-3</sup> s<sup>-1</sup> sr<sup>-1</sup>

The line emissivities of 10 emission lines are output by the model, including 5 rotational transitions of CO, the 158-µm forbidden transition of [C II], 2 forbidden transitions of [O I] and 2 forbidden transitions of [C I]. These lines are chosen to be those that dominate the cooling of the neutral and molecular ISM over a wide range of pressures. The lines are listed in Table 3.1. j(X) can be easily converted into erg s<sup>-1</sup> sr<sup>-1</sup> per H by simply dividing it by  $n_{\rm H}$ .

| Species | Transition                            | Wavelength (µm) | Einstein A coefficient $(s^{-1})$ | Critical density (cm <sup>-3</sup> ) |
|---------|---------------------------------------|-----------------|-----------------------------------|--------------------------------------|
| СО      | $J = 1 \rightarrow 0$                 | 2600.8          | $7.2 	imes 10^{-8}$               | $1.1 	imes 10^3$                     |
| СО      | $J = 2 \rightarrow 1$                 | 1300.4          | $6.9	imes10^{-7}$                 | $6.7 	imes 10^3$                     |
| СО      | $J = 3 \rightarrow 2$                 | 867.0           | $2.5 	imes 10^{-6}$               | $2.1 	imes 10^4$                     |
| СО      | $J = 4 \rightarrow 3$                 | 650.3           | $6.1 	imes 10^{-6}$               | $4.4	imes10^4$                       |
| СО      | $J = 5 \rightarrow 4$                 | 520.2           | $1.2 	imes 10^{-5}$               | $7.8	imes10^4$                       |
| CII     | ${}^2P_{3/2} \to {}^2P_{1/2}$         | 157.7           | $2.4	imes10^{-6}$                 | $2.7 	imes 10^3$                     |
| От      | ${}^{3}P_{0} \rightarrow {}^{3}P_{1}$ | 63.2            | $8.95	imes10^{-5}$                | $9.7 	imes 10^5$                     |
| От      | ${}^{3}P_{1} \rightarrow {}^{3}P_{2}$ | 145.5           | $1.7	imes10^{-5}$                 | $1.5 	imes 10^5$                     |
| Ст      | ${}^{3}P_{1} \rightarrow {}^{3}P_{0}$ | 370.4           | $2.7	imes10^{-7}$                 | $9.3 	imes 10^{2}$                   |
| Ст      | $^{3}P_{2} \rightarrow ^{3}P_{1}$     | 609.1           | $7.9	imes10^{-8}$                 | $4.9 	imes 10^2$                     |

TABLE 3.1: List of emission lines in the model. Data taken from Tielens (2005).

# 3.4 Assumptions of the model

#### 3.4.1 Chemical equilibrium

The lifetime of a typical interstellar cloud is  $\sim 2 \times 10^6$  years (Larson (1994)), which is longer than the chemical timescale (timescale to cycle through the gas through molecules):  $\tau_{chem} = x_{O,g}/\zeta_H \simeq 3 \times 10^5$  years (Tielens (2005)), where  $\zeta_H$  is the total CR ionisation rate of per hydrogen nucleus (see Section 3.9.1). In addition, in the cold neutral medium, the cooling timescale  $\tau_{cool} = 3k_BT/2n\Lambda \lesssim 5 \times 10^3$  years. Therefore, I assume that the thermodynamic state and chemical state of the gas is stable over long periods of time. Non-equilibrium chemistry show moderate effects (Penãloza et al. (2017)), which should be taken into account in a complete model. However, because of the context of developing a semi-analytical model for clouds in Chapter 5, non-equilibrium effects are disregarded here. Assuming the gas is in chemical equilibrium under the conditions specified (the ISRF and the thermal state of the gas), the number density of individual chemical species is solved by balancing the total formation rate and total destruction rate due to all (considered) chemical pathways involving that species.

## 3.5 Structure of the code

The overall idea of the code is to first solve for the number densities of all chemical species under some trial assumption for *T*, since the calculation of quantities such as the gas cooling rates and the line emissivities requires the values of the number densities of the chemical species and *T*. To solve for the number densities of the species, one needs to track the abundances of the species through a chemical network, which includes all chemical reactions that are considered and their associated reaction rates. The choice of which chemical reactions to include is an important one, since I want to include enough reactions to incorporate the most important cooling processes in interstellar gas. The model aims to predict the species that produce the cooling lines which are observed to dominate the gas cooling. However, including too many reactions will make the model too complicated and increase the computation time significantly. The code includes a total of 20 chemical reactions that describe the chemistry of the 12 chemical species in the model. Section **3.6** describes the chemical reactions in detail. The chemistry part of the code, together with the PE heating model described in Chapter **2**, forms the backbone of my ISM code.

The strategy for solving for the unknown quantities is to identify the most important quantities where knowing these quantities allows one to calculate the values of all other quantities analytically. It was discovered that there are 5 quantities that fulfil this condition: T,  $n_{\rm H}$ ,  $n_{\rm e}$ ,  $f_{\rm H_2}$  and  $n_{\rm C^+}$  (see Appendix **B** for the analytic equations for the number densities of all species). Therefore, in order to solve for the quantities in a semi-analytical way, 5 nested loops (or iterations) are set up. From the outermost loop to the innermost loop, they are T,  $n_{\rm H}$ ,  $n_{\rm e}$ ,  $f_{\rm H_2}$  and  $n_{\rm C^+}$ . All loops must be solved numerically . To move into the inner loops, one has to assume *a priori* values (trial values) from the outer loops. These values are initial guesses to the actual solutions and they facilitate the solve for the actual solutions. For example, one must provide trial values of T,  $n_{\rm H}$ ,  $n_{\rm e}$ , and  $f_{\rm H_2}$  in order to solve for  $n_{\rm C^+}$ . Once  $n_{\rm C^+}$  is solved, the actual solution of  $n_{\rm C^+}$  is propagated outwards so that the actual solution of  $f_{\rm H_2}$  can be found, and so that the cooling and heating rates can be compared to see whether thermal equilibrium has been reached. To see why T is placed in the outermost loop, consider the rate coefficient of a typical chemical reaction in the ISM:

$$k = \alpha \left(\frac{T}{300}\right)^{\beta} e^{-\gamma/T}, \qquad (3.4)$$

where  $\alpha$ ,  $\beta$  and  $\gamma$  are constants and *T* is in K. As *T* influences the chemical reaction rates and the photoelectric heating rate, it is a crucial parameter in the model and so is solved in the outermost loop. The fact that *T* is the most difficult quantity to solve

numerically is also the reason why T is solved in the outermost iteration. Within each loop, the actual solution of the quantity is numerically solved using the "binary chop method", which will be discussed in Section 3.5.1.

The 5 loops, from the outermost loop to the innermost loop, are as follows:

1. Finding the value of *T* 

*T* is solved from the thermal balance equation, with the assumption of thermal equilibrium:

$$\Gamma_{\rm tot} = \Lambda_{\rm tot},\tag{3.5}$$

where  $\Gamma_{tot}$  is the total gas heating rate in erg cm<sup>-3</sup> s<sup>-1</sup> and  $\Lambda_{tot}$  is the total gas cooling rate in erg cm<sup>-3</sup> s<sup>-1</sup>. There are three channels of gas heating: photoelectric heating on dust grains, which is discussed in Chapter 2, cosmic ray heating, and heating due to gas-dust interactions. The final term only exists if the temperature of dust grains is higher than the gas temperature, which is not usually the case in the cold neutral medium (CNM), but it exists in higher density environments such as molecular clouds, as shown in Section 3.12. Interstellar gas can be cooled by line emission and by gas-dust interactions if the dust is cooler than the gas. For cooling by line emission, cooling by lines of C II, O I, CO and C I are considered. Therefore, Equation 3.5 can be written as

$$\Gamma_{\rm PE} + \Gamma_{\rm CR} = \Lambda_{\rm C\,II} + \Lambda_{\rm O\,I} + \Lambda_{\rm CO} + \Lambda_{\rm C\,I} + \Lambda_{\rm gas-dust},\tag{3.6}$$

where  $\Gamma_X$  is the heating rate due to process *X* and  $\Lambda_X$  is the cooling rate due to process *X*. If  $\Lambda_{gas-dust} < 0$ , this term becomes a gas heating rate.

For low thermal pressures ( $P_{\text{therm}}/k_B \lesssim 5 \times 10^3 \text{ K cm}^{-3}$ ), the code may find two valid solutions for *T*. In this case the higher temperature solution, which often has  $T \sim 1000$  K, is discarded since it corresponds to the thermally unstable equilibrium, which lies between the thermally stable temperature solutions of the CNM and the warm neutral medium (see Draine (2011) and Section 3.6). As my code is catered to solving the thermal balance in the CNM (including diffuse atomic clouds and molecular clouds), only the lower temperature solution, which corresponds to typical gas temperatures in the CNM, is output from the code.

#### 2. Finding the value of $n_{\rm H}$

The ideal gas law is used to relate the thermal pressure  $P_{\text{therm}}$ ,  $n_{\text{H}}$ ,  $f_{\text{H}_2}$  and T:

$$P_{\text{therm}} = nk_{\text{B}}T \approx (n_{\text{H}\,\text{I}} + n_{\text{H}_2} + n_{\text{He},\text{g}})k_{\text{B}}T$$
 (3.7)

$$= \left(1 - \frac{f_{\rm H_2}}{2} + x_{\rm He,g}\right) n_{\rm H} k_{\rm B} T, \qquad (3.8)$$

where *n* is the total gas density and  $n_{\text{He},g} = n_{\text{He}} + n_{\text{He}^+}$ . For known input parameter  $P_{\text{therm}}$  and trial  $f_{\text{H}_2}$ ,  $n_{\text{H}}$  is given by the above equation. However, these trial values of  $f_{\text{H}_2}$  and  $n_{\text{H}}$  may not satisfy the H<sub>2</sub> balance equation (see Step 4), so one needs to iterate in the inner loops to find the true solutions of  $f_{\text{H}_2}$  and  $n_{\text{H}}$ .

3. Finding the value of  $n_{\rm e}$ 

 $n_{\rm e}$  is solved by considering the ionisation balance equation:

$$n_{\rm e} = n_{\rm H^+} + n_{\rm H_2^+} + n_{\rm H_2^+} + n_{\rm He^+} + n_{\rm C^+}.$$
(3.9)

This is important for the self-consistent treatment of PE heating, especially in the role of other sources of ionisation, such as CRs.

4. Finding the value of  $f_{\rm H_2}$ 

The formation of  $H_2$  on dust grains is the main formation pathway of  $H_2$ , which is the topic of Section 3.7. The main destruction pathways of  $H_2$  include the photodissociation due to FUV photons, CR ionisation and the reaction between  $H_2$  and  $C^+$  (see Appendix B.2). The balance equation of  $H_2$  is

$$R_{\rm H_2}n_{\rm H_1}n_{\rm H} + k_{14}n_{\rm H_1}n_{\rm H_2^+} + k_{12}n_{\rm e}n_{\rm H_3^+} = \left[ (k_4 + k_5 + k_2) + k_{15}n_{\rm H_2^+} + k_{16}n_{\rm C^+} \right] n_{\rm H_2}.$$
(3.10)

The full derivation of this equation, together with the balance equations of other species, can be found in Appendix B. Since  $f_{H_2}$  depends on  $n_e$  (see Equation B.7),  $f_{H_2}$  is placed in an inner loop compared to  $n_e$ .

5. Finding the values of  $n_{C^+}$ ,  $n_C$  and  $n_{CO}$ 

The number densities of carbon-containing species are solved by considering the equation for the total carbon abundance in the gas phase:

$$x_{C,g} = x_{C^+} + x_C + x_{CO}.$$
 (3.11)

A cubic equation in  $n_{\rm CO}$  can be written with coefficients containing *T*,  $f_{\rm H_2}$ ,  $n_{\rm H}$ ,  $n_{\rm e}$  and  $n_{\rm C^+}$  (see Equation B.34 in Appendix B).  $x_{\rm C}$  can be simply found by  $x_{\rm C,g} - x_{\rm C^+} - x_{\rm CO}$ .  $x_{\rm C^+}$  can be found by using the "binary chop" method iteratively so that the Equation 3.11 holds within some tolerance value.

#### 3.5.1 The "binary chop" algorithm

The binary chop algorithm aims to search for the solution(s) to the equation by reducing the search range by half iteratively until one (or more) solution(s) are found. The search ends when the relative error between both sides of the equation is within the tolerance value - 1%. It is discovered that for every loop except for *T*, only one solution is found, so I do not have to worry about having multiple solutions.

#### 3.5.2 Theoretical reduction in the number of search loops

In principle, the number of search loops can be reduced to 4 if one implements the following method.

- 1. Search for *T* (trial *T*).
- 2. Search for  $f_{H_2}$  (trial  $f_{H_2}$ ). The value of  $n_H$  can be known immediately from Equation 3.8.
- Search for x<sub>e</sub>. If *T*, *f*<sub>H2</sub>, *n*<sub>H</sub> and *n*<sub>e</sub> are known, *n*<sub>He<sup>+</sup></sub> can calculated using B.12.
   *n*<sub>H2<sup>+</sup></sub> can calculated using B.4. Together with *n*<sub>H2<sup>+</sup></sub>, *n*<sub>H<sup>+</sup></sub> can be calculated using B.10.
- 4. Search for  $x_{C^+}$ .  $x_{CO}$  can be found by solving the cubic equation in  $n_{CO}$  (Equation B.34).  $x_C$  can be easily found from Equation 3.11. Similarly,  $x_O$  can be easily found by subtracting  $x_{CO}$  from the total gas-phase oxygen abundance (Equation B.26). Hence the abundances of all chemical species are found.

One then finds *T* for which  $\Gamma_{\text{tot}}(T) = \Lambda_{\text{tot}}(T)$ . The following section describes the modelling of the chemistry in detail.

## 3.6 Modelling the chemistry in the neutral and molecular ISM

The neutral and molecular ISM refers to the phases in the ISM which contain hydrogen in neutral atomic form (H I) or molecular form (H<sub>2</sub>). Referring to Table 1.1, the neutral medium can be sub-divided into the cold neutral medium (CNM) and the warm neutral medium (WNM). The WNM is significantly hotter than the CNM, with gas temperatures between 6000 K and 10,000 K. Having a typical gas temperature of ~80 K, the CNM is both cooler and denser than the WNM. For the purposes in this thesis, the CNM will be the main focus in the neutral ISM. Molecular clouds contain mostly H<sub>2</sub> and they are cooler and denser than the CNM. The gas temperature (*T*) in their cores can reach as low as 10 K and the hydrogen nuclei density ( $n_{\rm H}$ ) can exceed 10<sup>5</sup> cm<sup>-3</sup> in their cores (Bergin et al. (1997)).

A class of objects where the transition from atomic phase to molecular phase is demonstrated clearly is photodissociation regions (PDRs). PDRs are regions where FUV photons dominate the energy balance or chemistry of the gas (Tielens (2005)). Figure 3.2 shows the chemical structure of a typical photodissociation region where the x-axis is the hydrogen column density ( $N_{\rm H}$ ) and the y-axis is the chemical abundance of different species. Regions with higher  $N_{\rm H}$  are denser, colder and have

higher optical depths. Thus, they have weaker FUV radiation fields. The transition from atomic phase to molecular phase can be clearly seen. The plot also shows the variation of the abundances of 3 major carbon-containing species ( $C^+$ , C and CO) through the PDR.



FIGURE 3.2: Results from a photodissociation region model with  $n_{\rm H} = 100 \text{ cm}^{-3}$  and  $G_0 = 1$ . The data was from Neufeld, Wolfire, and Schilke (2005) and figure reproduced with permission from Snow and McCall (2006).

#### 3.6.1 Glassgold and Langer (1974) model

As mentioned in Chapter 2, the electron density ( $n_e$ ) is a crucial parameter in photoelectric heating since it determines the charge states of interstellar dust grains, which influence the photoelectric yield and hence the photoelectric heating rate. The first idea is to see if a simple chemical model that provides analytical expressions for  $n_e$ and the abundances of other chemical species exists in the literature. Glassgold and Langer (1974) (GL74) contains a very simple chemical network that includes analytical expressions for  $n_e$  and other species. However, this model contains H, H<sub>2</sub>, H<sup>+</sup>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, He, C<sup>+</sup>, C, and electrons, but it does not contain O and CO. Therefore, the GL74 model is used as the backbone of the chemical model, and 5 reactions are added into the model so that the model also contains O and CO. The GL74 model is first described below.

#### 3.6.2 Hydrogen chemistry



FIGURE 3.3: Chemical network of hydrogen species used in Glassgold and Langer (1974) and this model

Figure 3.3 shows the reaction network of the hydrogen species considered in GL74, which is used in full in the chemical model in this thesis. The reactions are explained as follows:

1. H<sub>2</sub> formation on grains  $(H + H \longrightarrow H_2)$ :

In principle, H<sub>2</sub> molecules can be formed from the radiative association of two hydrogen atoms in the gaseous phase of the ISM. However, H<sub>2</sub> has a very low rate coefficient for radiative association,  $10^{-29}$  cm<sup>3</sup> s<sup>-1</sup> (Duley and Williams (1984)), since the proto-molecule has to make a spin forbidden transition to the ground electronic state from a dissociative state. Therefore, the formation of H<sub>2</sub> in the gaseous phase of the ISM is very inefficient. Jura (1975) found that the rate coefficient of H<sub>2</sub> formation  $R_{H_2}$  in diffuse clouds to be  $10^{-17}$ cm<sup>3</sup> s<sup>-1</sup> <  $R_{H_2}$  <  $3 \times 10^{-17}$ cm<sup>3</sup> s<sup>-1</sup>. To explain the observed H<sub>2</sub> formation rate, van de Hulst (1949) proposed that interstellar dust grains act as a catalyst for H<sub>2</sub> formation in the ISM. This idea was later developed into a theory by Gould and Salpeter (1963), solving the H<sub>2</sub> formation. The process of H<sub>2</sub> formation on dust grains will be discussed in detail in Section 3.4.

2. Photodissociation of H<sub>2</sub> (H<sub>2</sub> +  $\gamma \rightarrow$  2H): H<sub>2</sub> molecules can be dissociated by FUV photons. The rate coefficient for this process, when converted in terms of *G*<sub>FUV</sub> defined in Section 2.5.1, is *k* =  $4.92 \times 10^{-11} G_{FUV} \text{ s}^{-1}$  (see Appendix B).

3. Cosmic ray ionisation of H (H + CR  $\rightarrow$  H<sup>+</sup> + e<sup>-</sup> + CR):

When a cosmic ray particle impacts with a hydrogen atom, the hydrogen atom is ionised. This ionisation process creates  $H^+$  (which is simply a proton) and an electron. This ionisation process also causes some kinetic energy in the cosmic ray particle to be transferred to the kinetic energy of the electron, which thermalises with other gas particles via inelastic collisions. Cosmic rays can heat the gas in the ISM in this way, which is the topic of Section 3.9.

- Cosmic ray ionisation of H<sub>2</sub> (H<sub>2</sub> + CR → H<sub>2</sub><sup>+</sup> + e<sup>-</sup> + CR): Similar to H<sub>1</sub>, H<sub>2</sub> is ionised during their collisions with cosmic ray particles. This process often produces H<sub>2</sub><sup>+</sup> and an electron; however, two H atoms and an electron may be formed. Cosmic ray heating also occurs in this process.
- Charge exchange between H and H<sub>2</sub><sup>+</sup> (H<sub>2</sub><sup>+</sup> + H → H<sub>2</sub> + H<sup>+</sup>): The positive charge of H<sub>2</sub><sup>+</sup> can be transferred to H during the collision between H<sub>2</sub><sup>+</sup> and H. H<sub>2</sub> and H<sup>+</sup> are formed in this process.
- 6. Ion-molecule reaction between  $H_2^+$  and  $H_2$   $(H_2^+ + H_2 \longrightarrow H_3^+ + H)$ : When  $H_2^+$  reacts with  $H_2$ ,  $H_3^+$  and H are formed during the process.

#### 3.6.3 Helium chemistry

Compared to the hydrogen species, the chemical reactions involving helium in the GL74 model are much simpler. Helium atoms are ionised by cosmic rays and helium ions (He<sup>+</sup>) recombine with electrons to form helium atoms:

$$He + CR \longrightarrow He^+ + e^- + CR,$$
 (3.12)

$$\mathrm{He^{+} + e^{-} \longrightarrow He + \gamma}.$$
 (3.13)

He<sup>+</sup> may also react with CO:

$$\mathrm{He^{+}} + \mathrm{CO} \longrightarrow \mathrm{He} + \mathrm{C^{+}} + \mathrm{O.}$$
 (3.14)

However, it is assumed that the abundance of He<sup>+</sup> is so low that this reaction, as a destruction pathway of CO, is negligible compared to the photodissociation of CO. This reaction becomes important in environments with high ionisation fraction, but for the purposes of this model, this reaction is not included in the chemical network.

#### 3.6.4 Carbon chemistry

In the GL74 model, carbon atoms (C) are ionised by FUV photons to form C<sup>+</sup> and electrons:

$$C + \gamma \longrightarrow C^+ + e^-. \tag{3.15}$$

C<sup>+</sup> and electrons recombine to form C radiatively:

$$C^+ + e^- \longrightarrow C + \gamma. \tag{3.16}$$

#### 3.6.5 Expanding the GL74 model

As described in Section 3.6.1, 5 extra reactions are added to the GL74 chemical network to incorporate O and CO. The 5 extra reactions are:

$$C^+ + H_2 \longrightarrow CH_2^+, \tag{3.17}$$

$$CH + O \longrightarrow CO + H$$
, (3.18)

$$CO + \gamma \longrightarrow C + O,$$
 (3.19)

$$CH + \gamma \longrightarrow C + H$$
, (3.20)

$$C + H_3^+ \dashrightarrow CH_2^+ \dashrightarrow CH.$$
(3.21)

Figure 3.4 shows the chemical network of carbon-containing species in the expanded chemical model.



FIGURE 3.4: Chemical network of carbon-containing species in the expanded chemical model

The formation and destruction of CO in the model follows the approach given in Nelson and Langer (1997). C<sup>+</sup> reacts with H<sub>2</sub> to form  $CH_2^+$ , which is then rapidly converted to CH by its reaction with H<sub>2</sub> and dissociative recombination with e<sup>-</sup>. The newly formed CH either reacts with O to form CO or is photodissociated by FUV photons. Therefore, the concentrations of CH and  $CH_2^+$  are negligible and these

species are not tracked in this model. A list of all reactions used in the model as well as their rate coefficients can be found in Appendix **B**.

CO can also be formed from the OH route:

$$OH + C \longrightarrow CO + H.$$
 (3.22)

From arguments involving rate coefficients, the formation of CO from the CH/CH<sub>2</sub><sup>+</sup> route is more important than the OH route at low gas temperatures (T < 30 K) and high gas densities ( $n_{\rm H} > 100$  cm<sup>-3</sup>) (Langer (1976)). Therefore, when using my model to model molecular clouds, it is appropriate to omit the formation of CO from the OH route. Other models also consider the formation of CO via HCO<sup>+</sup>:

$$HCO^+ + e^- \longrightarrow CO + H.$$
 (3.23)

However, since HCO<sup>+</sup> requires CO<sup>+</sup> to form (CO<sup>+</sup> + H<sub>2</sub>  $\rightarrow$  HCO<sup>+</sup> + H), which requires OH to form (C<sup>+</sup> + OH  $\rightarrow$  CO<sup>+</sup> + H) (Klessen and Glover (2016)), the formation of CO from HCO<sup>+</sup> can be viewed as a branch in the OH route.

# **3.7** Formation of H<sub>2</sub> on dust grains

It is currently understood that most of the  $H_2$  in the interstellar medium is made on dust grains by the interaction of two neutrally charged hydrogen atoms that become trapped on the surface of a dust grain (Vidali (2013)). Several mechanisms have been proposed as the mechanism in which  $H_2$  forms on the surfaces of a wide variety of solids (Wakelam et al. (2017)). These include the Langmuir-Hinselwood mechanism, the Eley-Rideal mechanism, and the "hot atom" mechanism (Kolansinski (2008)).

In the Langmuir-Hinshelwood mechanism, gas phase atoms first become accommodated on the surface and then encounter each other via diffusion and react. The resulting molecule might or might not leave the surface, depending on how the energy gained in the reaction is partitioned.

I follow the approach by Cazaux and Tielens (2002) (CT02), whose model of H<sub>2</sub> formation on grain surfaces is based on the Langmuir-Hinshelwood mechanism. In this model, the mobility of hydrogen atoms is due to both quantum tunnelling and thermal diffusion, and the hydrogen atoms can bind to the grain surface in a physisorption site or a chemisorption site, which are two energetically different sites. At low grain temperatures ( $T_d < 100$  K), H<sub>2</sub> formation mostly involves the migration of physisorbed H atoms.

#### **3.7.1** H<sub>2</sub> formation rate

Based on an analysis of the observations of H I and H<sub>2</sub> in the local diffuse clouds by the *Copernicus* satellite, Jura (1975) derived the formation rate of H<sub>2</sub> on dust grains, if assumed to be constant in interstellar clouds, to be  $3 \times 10^{-17} n_{\rm H} n_{\rm H1}$  cm<sup>3</sup> s<sup>-1</sup>. This was later confirmed by observations by the *Far Ultraviolet Spectroscopic Explorer* (FUSE) (Welsh et al. (2002)). However, this contained implicit assumptions about the grain model and the sticking coefficient. Referring to Cazaux and Tielens (2002), the H<sub>2</sub> formation rate on grains can be more properly written as

$$R_{\rm H_2} = \frac{1}{2} n_{\rm H\,I} \, v_{\rm H} \, n_{\rm d} \, \sigma_{\rm d} \, \epsilon_{\rm H_2} \, s_{\rm H}(T), \qquad (3.24)$$

where  $v_{\rm H}$  is the velocity of H atoms in cm s<sup>-1</sup>,  $n_{\rm d}$  is the number density of dust grains per H in cm<sup>-3</sup>,  $\sigma_{\rm d}$  is the cross section of the dust grain in cm<sup>-2</sup>,  $\epsilon_{\rm H_2}$  is the formation efficiency, and  $s_{\rm H}$  is the sticking coefficient of H atoms (see Section 3.7.3).

For a certain grain model, the  $H_2$  formation rate at gas temperature *T* can be rewritten as:

$$R_{\rm H_2}(T) = \sum_{i} \int_{a_{\rm max}(i)}^{a_{\rm min}(i)} \frac{1}{2} n_{\rm H} v_{\rm H}(T) n_{\rm d}(i,a) \sigma_{\rm d}(a) \epsilon_{\rm H_2}(i,T_{\rm d}) s_{\rm H}(T_{\rm d},T) da, \qquad (3.25)$$

where *i* is the grain composition, *a* is the grain radius and  $T_d$  is the grain temperature.  $T_d$  can be found by solving the energy balance of the grain (see Equation 3.35) and assuming a delta function for the  $T_d$  for a certain grain composition and grain size. Therefore,  $T_d$  can be written as  $T_d = T_d(u_v, i, a)$  in a certain ISRF.

#### 3.7.2 Formation efficiency

The method outlined CT02 is used to calculate the formation efficiency of H<sub>2</sub> on dust grains ( $\epsilon_{\text{H}_2}$ ). For  $T_{\text{d}} < 300$  K, it is formulated as:

$$\epsilon_{\rm H_2} = \left(1 + \frac{\mu F}{2\beta_{\rm H_2}} + \frac{\beta_{\rm H_P}}{\alpha_{\rm PC}}\right)^{-1},\tag{3.26}$$

where  $\mu$  is the fraction of newly formed H<sub>2</sub> molecules that stay on the surface, *F* is the flux of H atoms in monolayers per second, H<sub>P</sub> represents physisorbed H,  $\beta_i$  is the desorption rate of population *i*:  $\beta_i = \nu_i \exp(-E_i/k_BT_d)$ ,  $\nu_i$  is the frequency factor of species *i* perpendicular to the surface,  $E_i$  is the desorption energy of species *i*, and  $\alpha_{PC}$  is the mobility for a H atom that goes from a physisorbed site to a chemisorbed site. At very low grain temperatures ( $T_d < 10$  K), due to tunnelling, the high mobility of H atoms permits the recombination of incoming H atoms. Since the grain temperature is not high enough to allow evaporation and prevents further accretion of H atoms, the newly formed H<sub>2</sub> stays on the surface. In this regime, the formation efficiency reduces to  $\epsilon_{H_2} = (\mu F/2\beta_{H_2})^{-1}$ . At higher grain temperatures, hydrogen accretes into a physisorbed site but quickly drops into a chemisorbed well, so the last term has to be considered. It can be expressed as

$$\frac{\beta_{\rm H_P}}{\alpha_{\rm PC}} = \frac{1}{4} \left( 1 + \sqrt{\frac{E_{\rm H_C} - E_{\rm S}}{E_{\rm H_P} - E_{\rm S}}} \right)^2 \exp\left(-\frac{E_{\rm S}}{k_{\rm B}T_{\rm d}}\right). \tag{3.27}$$

These parameters were determined by experimental data and taken from Cazaux and Spaans (2004) (see Table 3.2). *F* is taken to be  $10^{-10}$  (monolayers per second). Figure 3.5 shows the formation efficiency on PAHs and silicate grains versus grain temperature.

 $\nu_{H_2} \; (s^{-1})$  $\nu_{\rm H_C} (\rm s^{-1})$ Composition  $E_{\mathrm{H}_{2}}\left(\mathrm{K}\right)$  $E_{\rm S}({\rm K})$  $E_{\mathrm{H}_{\mathrm{P}}}(\mathrm{K})$  $E_{\mathrm{H}_{\mathrm{C}}}(\mathrm{K})$ μ Silicate 340 200 650 30000  $2 \times 10^{12}$  $1 \times 10^{13}$ 0.3  $3 \times 10^{12}$  $2 imes 10^{13}$ 540 250 800 30000 Carbonaceous 0.4

TABLE 3.2: Parameters in the  $H_2$  formation model by Cazaux and Spaans (2004)



FIGURE 3.5: Formation efficiency versus grain temperature

From Figure 3.5, if the temperature of a PAH grain is lower than 10 K, hardly any H<sub>2</sub> is formed on the surface as the H<sub>2</sub> formation efficiency drops to 0. However, H<sub>2</sub> can form on silicate grains down to  $T_d = 6$  K.

#### 3.7.3 Sticking coefficient

The sticking coefficient (a probability) is defined as the ratio of the adsorption rate to the impingement rate of the gas particles on the surface (Winkler and Rendulic (1992)). Cazaux and Spaans (2004) provided a formulation of the sticking coefficient in terms of the gas temperature and dust temperature, and referenced Hollenbach and McKee (1979):

$$s_{\rm H} = \left[1 + 0.4 \left(\frac{T + T_{\rm d}}{100 \,\rm K}\right)^{1/2} + 0.2 \left(\frac{T}{100 \,\rm K}\right) + 0.08 \left(\frac{T}{100 \,\rm K}\right)^2\right]^{-1},\tag{3.28}$$

where  $T_d$  is the temperature of the dust grain. This sticking coefficient is calculated for each grain size and grain composition. Figure 3.6 shows the sticking coefficient versus gas temperature for different grain temperatures.



FIGURE 3.6: Sticking coefficient versus gas temperature for different grain temperatures

#### 3.7.4 Finding the grain temperature

The temperature of a dust grain  $T_d$  can be found by balancing the energy absorbed by the grain and the energy emitted by the grain. Considering the absorption characteristics of the grain, the energy absorbed by a grain of radius *a* is

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{abs}} = \pi a^2 c \int Q_{\mathrm{abs}}(a,\nu) \, u_{\nu}(\nu) \, \mathrm{d}\nu, \qquad (3.29)$$

whereas the energy emitted by the grain is

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{emiss}} = 4\pi a^2 \langle Q_{\mathrm{abs}} \rangle_{T_{\mathrm{d}}}(a) \,\sigma_{\mathrm{SB}} T_{\mathrm{d}}^4,\tag{3.30}$$

where  $\sigma_{SB}$  is the Stefan-Boltzmann constant,  $Q_{abs}$  is the absorption coefficient of the grain (depends on grain size and photon frequency). The quantity  $\langle Q_{abs} \rangle_{T_d}$  is the Planck-averaged absorption coefficient:

$$\langle Q_{\rm abs} \rangle_{T_{\rm d}} = \frac{\int B_{\nu}(T_{\rm d}) Q_{\rm abs}(a,\nu) d\nu}{\int B_{\nu}(T_{\rm d}) d\nu},\tag{3.31}$$

where  $B_{\nu}(T)$  is Planck's function. For the ease of calculation, the fitting functions from Draine (2011), which agree very well at  $T_{\rm d} \leq 10^2$  K with the Planck averages, were used to calculate  $\langle Q_{\rm abs} \rangle_{T_{\rm d}}$ :

$$\langle Q_{\rm abs} \rangle_{T_{\rm d}} \approx \begin{cases} 1.3 \times 10^{-6} \left(\frac{a}{0.1 \,\mu{\rm m}}\right) \left(\frac{T_{\rm d}}{{\rm K}}\right)^2 & (\text{silicate}). \\ 8 \times 10^{-7} \left(\frac{a}{0.1 \,\mu{\rm m}}\right) \left(\frac{T_{\rm d}}{{\rm K}}\right)^2 & (\text{graphite}). \end{cases}$$
(3.32)

In the calculation of the energy absorption rate of the grain, the input SED  $u_{\nu}(\nu)$  ranges from 912 Å to 10 µm. In the slab calculations in Section 3.12, the input SED in the infrared at  $\tau_{\rm B}$  is the infrared part of the Mathis ISRF at  $\tau_{\rm B}$ , scaled by a constant  $G_{\rm ini}$ .

The energy exchange rate due to the collisions between species i in the gas and a single dust grain is given by

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{coll},i} = \left[n_i \left(\frac{8k_\mathrm{B}T}{\pi m_i}\right)^{1/2} \pi a^2\right] 2k_\mathrm{B}(T-T_\mathrm{d})\alpha_{ij},\tag{3.33}$$

where  $m_i$  is the mass of a molecule of species *i* and  $\alpha_{ij}$  the thermal accommodation coefficient for species *i* and a dust composition *j*. H, H<sub>2</sub> and He are the considered species in this model. If this (d*E*/d*t*) term is positive, heat is transferred from species *i* in the gas to the dust. The approximate values of  $\alpha$  for H and H<sub>2</sub> are taken from Burke and Hollenbach (1983), while for helium atoms a value of 0.6 is assumed for both silicate grains and graphite/PAH grains. These values are tabulated in Table 3.3.

| collision partner | grain composition | α   |
|-------------------|-------------------|-----|
| Н                 | silicate          | 0.6 |
| Н                 | graphite/PAH      | 0.8 |
| H <sub>2</sub>    | silicate          | 0.6 |
| H <sub>2</sub>    | graphite/PAH      | 0.7 |
| He                | silicate          | 0.6 |
| He                | graphite/PAH      | 0.6 |

TABLE 3.3: Thermal accommodation coefficient ( $\alpha$ ) used in the model. Values for H and H<sub>2</sub> are taken from Burke and Hollenbach (1983).

The total energy exchange rate due to collisions between the gas and dust grains per grain is:

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{coll}} = \sum_{i} \left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{coll},i}.$$
(3.34)

The thermal balance of a given dust grain is

$$\left(\frac{dE}{dt}\right)_{abs} + \left(\frac{dE}{dt}\right)_{coll} = \left(\frac{dE}{dt}\right)_{emiss}.$$
(3.35)

This equation is numerically solved for  $T_d$  for each grain size and grain composition within the fourth loop (the loop solving for  $f_{H_2}$ ), since  $f_{H_2}$  is required to know  $n_{H_1}$ and  $n_{H_2}$  for the energy transfer rate due to collisions. This is important for calculating the H<sub>2</sub> formation rate.

# 3.8 Gas cooling/heating due to gas-dust interaction

From the perspective of the gas, the gas cooling rate due to collisions between the gas and dust grains with composition j is

$$\Lambda_{\text{gas-dust},j} = \sum_{i} \int n_i \left(\frac{8k_{\text{B}}T}{\pi m_i}\right)^{1/2} \alpha_{ij} \, 2k_{\text{B}}(T - T_{\text{d},j}) \, \sigma_{\text{d},j}, \left(\frac{\mathrm{d}n_{\text{d},j}}{\mathrm{d}a_j}\right) \mathrm{d}a_j \tag{3.36}$$

$$=\sum_{i}\int n_{i}\left(\frac{8k_{\mathrm{B}}T}{\pi m_{i}}\right)^{1/2}\alpha_{ij}\,2k_{\mathrm{B}}(T-T_{\mathrm{d},j})\,\pi a_{j}^{2}\left(\frac{\mathrm{d}n_{\mathrm{d},j}}{\mathrm{d}a_{j}}\right)\mathrm{d}a_{j},\qquad(3.37)$$

where  $\sigma_{d,j}$  is the collisional cross-section of the dust grain. The total gas cooling rate due to gas-dust interactions is then

$$\Lambda_{\text{gas-dust}} = \sum_{j} \Lambda_{\text{gas-dust},j}.$$
(3.38)

This term becomes a heating rate if there is net energy transfer from the dust to the gas (it has a negative value). This occurs when the dust temperature is higher than the gas temperature in general, which can happen in highly obscured regions in molecular clouds.

# 3.9 Cosmic ray heating

The main process by which CRs transfer their kinetic energy to interstellar gas is through ionising the gas particles (mainly H, H<sub>2</sub> and He). On average,  $\sim$ 30 eV of energy is transferred from the energetic CR particle to the ejected electron when the CR particle ionises the hydrogen or helium molecule. The 30 eV is either deposited into the gas as heat by thermalising with the gas particles or initiating further ionisations. I follow the formulation given by Glassgold, Galli, and Padovani (2012) (GGP12) to calculate the cosmic ray heating rate, which is described in the following.

#### 3.9.1 CR heating based on GGP12's formulation

GGP12 based their studies on Dalgarno, Yan, and Liu (1999) (DYL99) on the heating efficiency of fast-moving electrons in pure H gas, pure H<sub>2</sub> gas and H-He mixture.

The heating energy per ion pair *Q* due to collisions with H and H<sub>2</sub> is

$$Q = \frac{x_{\rm H}Q({\rm H}) + x({\rm H}_2)Q({\rm H}_2)}{x_{\rm H} + x_{\rm H_2}},$$
(3.39)

where  $x_{\rm H} + 2x_{\rm H_2} = 1$ . Since  $f_{\rm H_2} = 2n_{\rm H_2}/n_{\rm H}$ , the equation becomes

$$Q = \frac{(1 - f_{\rm H_2})Q({\rm H}) + f_{\rm H_2}Q({\rm H_2})/2}{1 - f_{\rm H_2}/2}.$$
(3.40)

The volumetric rate of ion-pair production is  $\zeta_H n_H$ , where  $\zeta_H$  is the total CR ionisation rate per H nucleus. Thus, the volumetric heating rate in erg cm<sup>-3</sup> s<sup>-1</sup> is

$$\Gamma_{\rm CR} = Q \,\zeta_{\rm H} \, n_{\rm H},\tag{3.41}$$

where  $\zeta_{\rm H}$  is defined as

$$\zeta_{\rm H} = (1 - f_{\rm H_2})\zeta_{\rm H\,I} + f_{\rm H_2}\zeta_{\rm H_2}/2,\tag{3.42}$$

where  $\zeta_{H_1}$  and  $\zeta_{H_2}$  are the total ionisation rate of H<sub>I</sub> and H<sub>2</sub> respectively, as defined in Section 3.2.

In atomic regions, the dominant heating process is elastic scattering. Q(H) can be estimated using Equation 14 and Table 7 in DYL99. The heating efficiency in a pure

HI gas is

$$\eta = 1 + \frac{\eta_0 - 1}{1 + Cx_e^{\alpha'}}$$
(3.43)

where  $x_e$  is the ionisation fraction. Assuming an incident electron energy *E* of 30 eV, the parameters in a pure H I gas are  $\eta_0 = 0.255$ ,  $\alpha = 0.985$  and C = 164. Table 3.4 shows the variation of  $\eta$  with  $x_e$ .

TABLE 3.4: The variation of  $\eta$  with  $x_e$ , according to the formulation of Dalgarno, Yan, and Liu (1999)

 $x_{e}$ 

η

| $1 	imes 10^{-4}$  | 0.2688 |  |
|--------------------|--------|--|
| $3	imes 10^{-4}$   | 0.2942 |  |
| $1 \times 10^{-3}$ | 0.3697 |  |
| $3 \times 10^{-3}$ | 0.5152 |  |
| $1 \times 10^{-2}$ | 0.7298 |  |

The mean kinetic energy of a primary electron  $\langle E_e \rangle \approx 35$  eV is essentially independent of the energy of the CR particle (Draine (2011)). Therefore, the energy of the primary electron *E* can be assumed to be 35 eV. *Q*(H) is then:

$$Q(\mathbf{H}) = \eta E_{\mathbf{e}}.\tag{3.44}$$

#### **3.9.2** Calculation of $Q(H_2)$

GGP12 did their calculations with electron energy  $E_e = 1000$  eV. However, since the primary electron resulted from the ionisation of hydrogen by cosmic rays has an average energy of 35 eV (see above), for simplicity I did all calculations assuming that all primary electrons have an energy of 30 eV, as DYL99 tabulate the heating efficiencies starting from 30 eV.

According to GGP12, the heating in molecular regions is the sum of the effects from elastic collisions plus rotational excitation ( $Q_{el/rot}$ ), excitation of H<sub>2</sub> vibrational levels ( $Q_{vib}$ ), dissociation of H<sub>2</sub> ( $Q_{diss}$ ), and chemical heating ( $Q_{chem}$ ):

$$Q(H_2) = Q_{el/rot} + Q_{vib} + Q_{diss} + Q_{chem}.$$
(3.45)

The details of each term are described in Appendix C.

## 3.10 Cooling due to spontaneous emission lines

To calculate the collisional de-excitation rate of a species (not hydrogen), I consider H<sub>I</sub> and H<sub>2</sub> as the two dominant colliding species. Line de-excitation by electron impact is ignored because the ionisation fraction in the CNM is not high. Then the collisional de-excitation rate  $C_{\rm ul}$  (in s<sup>-1</sup>) can be calculated as

$$C_{\rm ul}(T) = n_{\rm H_2} \gamma_{\rm ul,H_2}(T) + n_{\rm H_1} \gamma_{\rm ul,H_I}(T), \qquad (3.46)$$

where  $\gamma_{ul,H_2}(T)$  is the coefficient of the collisional de-excitation of that species due to H<sub>2</sub>. It is dependent on the gas temperature and have units of cm<sup>3</sup> s<sup>-1</sup>. To estimate  $\gamma_{ul,H_2}$  for a particular temperature, I found the values of  $\gamma_{ul,H_2}$  at specific temperatures (e.g. 50 K) in the LAMDA database (Schöier et al. (2005)) and used linear interpolation to interpolate  $\gamma_{ul,H_2}$ .  $\gamma_{ul,H_1}$  was treated in a similar way.

The collisional excitation rate can be calculated by

$$C_{\rm lu} = \left(\frac{g_{\rm u}}{g_{\rm l}}\right) C_{\rm ul} \,\mathrm{e}^{-E_{\rm ul}/k_{\rm B}T},\tag{3.47}$$

where  $g_l$  and  $g_u$  are the degeneracies of the lower and upper levels respectively,  $E_{ul}$  is the energy difference between the levels. The transition rate from level *i* to level *j* (in s<sup>-1</sup>) is given by

$$R_{ij} = C_{ij} + A_{ij} + B_{ij}I_{\nu,ij}, ag{3.48}$$

where  $A_{ij}$  is the coefficient for spontaneous emission,  $B_{ij}$  is the stimulated excitation/deexcitation coefficient and  $I_{v,ij}$  is the specific radiation intensity at the frequency of the transition from level *i* to level *j*. If  $i - j \neq 1$ ,  $A_{ij} = 0$ . If  $|i - j| \neq 1$ ,  $B_{ij} = 0$ . See Appendix D for the relationship between  $A_{ij}$  and  $B_{ij}$ , and basic atomic physics of line emission. As mentioned in Section 3.2,  $I_{v,ij}$  is an input in my model. It can be supplied by a calling program computing radiative transfer of the object being modelled.

Assuming statistical equilibrium (hence using the principle of detailed balance) and considering the number density of the species in level *i*, the relationship between the number densities in levels *i* and *j* is given by

$$n_i \sum_{j \neq i}^k R_{ij} = \sum_{j \neq i}^k n_j R_{ji},$$
 (3.49)

where *k* is the total number of energy levels +1 (since the ground energy level is usually labelled as *E*<sub>0</sub>). Solving this equation, together with the constraint of  $\sum_{i=1}^{k} n_i = n$  gives the distribution of a particular species over the relevant energy levels.

Using the CO rotational lines as an example, I now illustrate the method of solving for the level populations by matrix inversion. The equations to consider are the constraint of the total number density of CO molecules in all energy levels considered:

$$n = \sum_{i=0}^{5} n_i, \tag{3.50}$$

where, for simplicity, *n* denotes  $n_{CO}$  and  $n_i$  denotes the number density of CO molecules in the J = i state. Since I consider CO rotational transitions up to  $J = 5 \rightarrow 4$ ,  $n_i$  is summed from i = 0 to i = 5.

To express Equations 3.48 and 3.49 in a compact way, I define the following matrices M (6 × 6), X (1 × 6) and N (1 × 6), with elements:

$$M_{ij} = \begin{cases} \sum_{j \neq i}^{5} R_{ij}, & \text{if } i < 5 \text{ and } i = j, \\ -R_{ji}, & \text{if } i < 5 \text{ and } i \neq j, \\ 1, & \text{if } i = 5. \end{cases}$$
(3.51)

$$X_i = n_i. ag{3.52}$$

$$N_i = \begin{cases} 0, & i < 5, \\ n, & i = 5. \end{cases}$$
(3.53)

Essentially, one wants to solve the matrix equation

$$MX = N. \tag{3.54}$$

This matrix equation can be easily solved by inverting *M*:

$$X = M^{-1}N. (3.55)$$

The emissivity of a particular species (in erg cm<sup>-3</sup> s<sup>-1</sup> sr<sup>-1</sup>) is due to spontaneous emission and it is given by

$$j_{ij} = \frac{h\nu_{ij}}{4\pi} n_i A_{ij},\tag{3.56}$$

where i > j and  $j_{ij}$  is the emissivity of the species due to spontaneous emission from level *j* to *i*. This assumes that the line profile function  $\phi_{\nu} = 1$ .

The cooling rate of CO in the  $J = i \rightarrow j$  line is

$$\Lambda_{\rm CO, ij} = h \nu_{ij} n_{\rm CO, i} A_{ij}. \tag{3.57}$$

For the cooling rate of species *X* other than CO in the transition  $u \rightarrow l$ , where u is the upper energy state and l the lower energy state, the cooling rate is

$$\Lambda_{X,\mathrm{ul}} = h \nu_{\mathrm{ul}} n_{X,\mathrm{u}} A_{\mathrm{ul}}.\tag{3.58}$$

# 3.11 Performance of the code

For a single calculation (with full PE heating calculation), the code (which is written in IDL) takes  $\sim$ 12 seconds to run on a typical laptop with a single processor. If the PE heating lookup table is used, the computation time is reduced to  $\sim$ 6 seconds. If the method described in 3.5.2 is used, in principle the time needed for the execution can be further reduced by a factor of a few.

## 3.12 Slab calculations

The following plots simulate a one-dimensional slab using Equation 2.23 to scale and attenuate the Mathis ISRF. Z' = 1 and  $F_{gr} = [0.7, 0.7]$  are used as the (relative) metallicity and dust depletion values. It is assumed that there is an external ISRF at one end of the slab (at  $\tau_{\rm B} = 0$ ) with an SED  $G_{\rm ini}$  times the Mathis ISRF. As  $\tau_{\rm B}$ increases, the column density of the dust increases linearly with  $N_{\rm H}$ , and the ISRF becomes more attenuated and reddened.

These plots are not meant to give physical solutions for real pressure-supported clouds. They are just a convenient way of depicting the dependence of solutions on arbitrary strength and colour of radiation fields.

The sampling of  $\tau_{\rm B}$  is from 0.0 to 8.0 with a step size of 0.2. The calculation starts at  $\tau_{\rm B} = 0$  with the unattenuated (external) radiation field. At each step, the code attempts to find a solution for the gas temperature within the search range 5 K  $\leq T \leq$  1200 K. If a valid solution for the gas temperature cannot be found, the code moves on to the next value of  $\tau_{\rm B}$ . This usually happens near the external boundary of the slab ( $\tau_{\rm B} \sim 0$ ), where sometimes when  $P_{\rm therm}$  is too low, the PE heating is too strong for the gas to be in thermal equilibrium ( $G_{\rm FUV}/P_{\rm therm}$  is too high, see Figure 3.7). The calculation continues with increasing  $\tau_{\rm B}$  until the gas temperature falls below 8 K, as mentioned in Section 3.3.

#### 3.12.1 Run 1: Low pressure, low ISRF and low CR ionisation rate

The following plots show the slab calculation when  $P_{\text{therm}} = 5 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$  and  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ . The thermal pressure is slightly higher than the median thermal pressure of the diffuse, neutral gas in the Galactic plane ( $P_{\text{therm}} = 3.6 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ) (Herrera-Camus et al. (2017)), but the conditions are similar to those in local cirrus clouds in the Milky Way. Notice that the calculations start at
$\tau_{\rm B} = 0.2$ , and end at  $\tau_{\rm B} = 2.6$  as the gas temperature becomes lower than 8 K beyond  $\tau_{\rm B} = 2.6$ . As expected, the molecular fraction and  $n_{\rm H}$  both increase with increasing  $\tau_{\rm B}$ . The electron density reaches a peak at  $\tau_{\rm B} \sim 2.2$  due to the rise in  $n_{\rm H}$ , then falls as the FUV ionisation rate of C decreases more rapidly than the increase in gas density. As Figure 3.9 shows, the electron abundance (ionisation fraction) drops rapidly after  $\tau_{\rm B} = 2.0$ .



FIGURE 3.7: Temperatures, molecular fraction, hydrogen density and electron density for  $P_{\text{therm}} = 5 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

Figure 3.8 shows the temperatures of grains of different sizes and compositions. The large grains are hotter than the small grains at high optical depths because the large grains have a much higher absorption efficiency at long wavelengths ( $\lambda > 1 \mu m$ ). The PAH grains have a higher absorption coefficient than silicate grains in the FUV (Draine (2011)), so they have a higher temperature than the silicate grains.



 $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3 \text{ K cm}^{-3}, G_{\text{ini}} = 1, \zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 3.8: Grain temperatures for  $P_{\text{therm}} = 5 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

Figure 3.9 shows the fractional abundances of the major species except He I. The main trends are that C<sup>+</sup> turns into C I and CO as  $\tau_B$  increases, and H I turns into H<sub>2</sub>, although most hydrogen is still in atomic form at  $\tau_B = 2.2$ .



 $P_{\rm therm}/k_{\rm B} = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 3.9: Abundances of major species except He I for  $P_{\text{therm}} = 5 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

Figure 3.10 shows the gas heating and gas cooling rates. PE heating dominates the heating, while cooling is dominated by the C II line for  $\tau_{\rm B} < 1.9$ . For  $\tau_{\rm B} \ge 1.9$ , C II cooling is overtaken by C I cooling. At  $\tau_{\rm B} \approx 2.1$ , as the gas becomes cooler than the

dust, there is a transition from net gas cooling due to gas-dust interactions to net gas heating due to gas-dust interactions.



 $P_{\rm therm}/k_{\rm B} = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 3.10: Gas heating and cooling rates for  $P_{\rm therm} = 5 \times 10^3 k_{\rm B} \, {\rm K} \, {\rm cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \, {\rm s}^{-1}$ 

Figure 3.11 shows the contributions of PE heating from FUV photons, NUV photons and optical photons. As the ISRF is not too reddened, the FUV photons dominate the PE heating. The CR heating is comparable to the heating by NUV photons and optical photons, but incomparable to the heating by FUV photons for  $\tau_{\rm B} < 2.0$ .



$$P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3 \text{ K cm}^{-3}, G_{\text{ini}} = 1, \zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$$

FIGURE 3.11: Components of gas heating for  $P_{\text{therm}} = 5 \times 10^3 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

Figure 3.12 shows the line emissivities. Out of the 5 CO lines, only the CO (1–0) and CO (2–1) lines are shown on this plot. The CO (1–0) line basically overlaps with the CO (2–1) line, because the gas density is always below the critical density for collisional excitation in both lines (see Table 3.1), while the gas temperature is always too high to influence excitation. The ratio between the emissivities of the CO lines can be expressed as

$$R_{21} = \frac{j_{\nu,(2-1)}}{j_{\nu,(1-0)}} = \frac{n_{\rm CO}f_2 \ h\nu_{21} \ A_{21}}{n_{\rm CO}f_1 \ h\nu_{10} \ A_{10}} \approx 19.2 \ \frac{f_2}{f_1},\tag{3.59}$$

where  $f_2$  and  $f_1$  are the fractions of CO molecules in the J = 2 and J = 1 states respectively. If  $R_{21}$  is approximately unity, this means  $f_2/f_1 \approx 1/19.2 = 0.052$ ; indeed, for  $0.2 \le \tau_B \le 2.6$ ,  $0.046 \le f_2/f_1 \le 0.053$ .



 $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 3.12: Line emissivities for  $P_{\rm therm} = 5 \times 10^3 k_{\rm B}$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17}$  s<sup>-1</sup>

Figure 3.13 shows all 5 CO lines together. Since a higher gas temperature is required to excite to higher rotational levels of CO, the higher transition lines are weaker than the lower transition lines.



FIGURE 3.13: Line emissivities for  $P_{\rm therm} = 5 \times 10^3 k_{\rm B}$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17}$  s<sup>-1</sup>

### 3.12.2 Run 2: High pressure, high ISRF and high CRIR

The following plots show the slab calculation when  $P_{\text{therm}} = 2 \times 10^6 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$  and  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ .  $n_{\text{H}}$  and the molecular fraction increase smoothly with increasing  $\tau_{\text{B}}$ . There is a peak in the electron density at  $\tau_{\text{B}} \approx 2.0$ . The left side is due to the increase in  $n_{\text{H}}$ , and the fall on the right side is due to the rapidly decreasing FUV photoionisation rate of C.



FIGURE 3.14: Temperatures, molecular fraction, hydrogen density and electron density for  $P_{\text{therm}} = 2 \times 10^6 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

Figure 3.15 shows the grain temperatures for this run. The grains are hotter than in Run 1 due to the higher external radiation field. PAH grains with a = 10 Å has a lower temperature than silicate grains at high optical depths, since the radiation field is very red there and silicate grains have an absorption peak around 10 µm (Draine (2011)).



 $P_{\rm therm}/k_{\rm B} = 2 \times 10^6 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 3.15: Grain temperatures for  $P_{\text{therm}} = 2 \times 10^6 \ k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

Figure 3.16 shows the abundance of major species (except He I). The overall trend of the carbon-containing species is the transition from C<sup>+</sup> to C to CO. C attains its maximum abundance at  $\tau \approx 2.8$  but it never substantially dominates the gas-phase carbon abundance.



 $P_{\rm therm}/k_{\rm B} = 2 \times 10^6 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 3.16: Abundances of major species for  $P_{\rm therm} = 2 \times 10^6 k_{\rm B} \, {\rm K} \, {\rm cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \, {\rm s}^{-1}$ 



 $P_{\text{therm}}/k_{\text{B}} = 2 \times 10^{6} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 3.17: Gas heating and cooling rates for  $P_{\rm therm} = 2 \times 10^6 k_{\rm B} \, {\rm K \, cm^{-3}}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \, {\rm s^{-1}}$ 

Figure 3.17 shows the gas heating and cooling rates for this run. The high CR ionisation rate makes CR heating to overtake PE heating at a relatively low optical depth ( $\tau_B \approx 2.8$ ). The large temperature difference between the gas and the dust makes the heating due to gas-dust energy transfer non-negligible at high optical depths, where the gas heating is dominated by CRs rather than by the PE effect.

Figure 3.18 shows the components of PE heating. The PE heating due to optical photons overtake the heating due to FUV photons at  $\tau_{\rm B} \approx 3.0$  and dominates the heating afterwards, as the radiation field becomes very red.



 $P_{\rm therm}/k_{\rm B} = 2 \times 10^6 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 3.18: Components of gas heating for  $P_{\text{therm}} = 2 \times 10^6 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

Figure 3.19 shows the line emissivities. The line emission is dominated by the C II 158-µm line below  $\tau_{\rm B} \approx 3.0$  and dominated by the CO (2-1) line afterwards. The O I 63-µm line is significant near  $\tau_{\rm B} = 0$  but drops rapidly with increasing optical depth due to the rapid decrease in gas temperature.



 $P_{\rm therm}/k_{\rm B} = 2 \times 10^6 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 3.19: Line emissivities for  $P_{\text{therm}} = 2 \times 10^6 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 



FIGURE 3.20: Line emissivities for  $P_{\text{therm}} = 2 \times 10^6 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

# 3.13 The importance of PE heating by optical photons

 $P_{\rm therm}/k_{\rm B} = 2 \times 10^4 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 1 \times 10^{-17} \text{ s}^{-1}$ PE (FUV) gas heating rate per H (erg  $s^{-1}$  H<sup>-1</sup>) PE (NUV)  $10^{-25}$ PE (optical) CR gas-dust  $10^{-26}$  $10^{-27}$  $10^{-28}$ 2 3 4 5 1  $au_{\mathsf{B}}$ 

FIGURE 3.21: Components of gas heating for  $P_{\text{therm}} = 2 \times 10^4 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 1 \times 10^{-17} \text{ s}^{-1}$ 

Figure 3.21 shows an example where PE heating by optical photons can be important. At  $\tau_{\rm B} = 3.8$ , heating due to gas-dust interactions is the strongest heating component, giving a heating rate of  $2.10 \times 10^{-27}$  erg s<sup>-1</sup> H<sup>-1</sup>. The PE gas heating rate due to optical photons, at  $1.52 \times 10^{-27}$  erg s<sup>-1</sup> H<sup>-1</sup>, is less than this and the FUV heating rate  $(1.71 \times 10^{-27} \text{ erg s}^{-1} \text{ H}^{-1})$ , but still comprises a substantial amount within the total gas heating rate.

# 3.14 Effects of cosmic rays on heating and chemistry

### 3.14.1 Increasing the ionisation fraction

A high CR ionisation rate produces extra free electrons as a by-product of the ionisation of gas particles (mainly hydrogen). This effect can be seen in Figure 3.22 and 3.23, where higher CR ionisation rate leads to higher ionisation fractions. The blue line represents the run with no cosmic rays ( $\zeta_p = 0 \text{ s}^{-1}$ ) and the ionisation of gas particles is only due to FUV photons. This line begins to dip beyond  $\tau_B = 1.5$  as there are fewer FUV photons available for ionisation. For  $\zeta_p \ge 1 \times 10^{-17} \text{ s}^{-1}$ , the extra free electrons change the ionisation balance of the gas by recombining with cations. For example, a high ionisation fraction shifts the equilibrium between C II and C I towards C I. As C I is a less effective coolant than C II, this has the effect of reducing the gas cooling and raising the gas temperature, as shown by the  $\zeta_p = 1 \times 10^{-15} \text{ s}^{-1}$  line in Figure 3.24. There is a turnover in gas temperature at  $\tau_B \approx 1.8$  as the free electrons produced by cosmic ray ionisation shift the C II–C I equilibrium towards C I.



FIGURE 3.22: Ionisation fraction for  $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ 



FIGURE 3.23: Electron density for  $P_{\rm therm}/k_{\rm B} = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ 



FIGURE 3.24: Gas temperature for  $P_{\rm therm}/k_{\rm B}=5 imes10^3$  K cm  $^{-3}$ ,  $G_{\rm ini}=1$ 

### 3.14.2 The "Catalyst" Effect

Figure 3.25 shows the change in PE heating rate per H under different CR ionisation rates, for low thermal pressure ( $P_{\text{therm}}/k_B = 5 \times 10^3 \text{ K cm}^{-3}$ ) and weak radiation field ( $G_{\text{ini}} = 1$ ). Compared to the run without CRs ( $\zeta_p = 0 \text{ s}^{-1}$ ), CR ionisation produces extra electrons make the dust grains more negatively charged (see Figures 3.26 and 3.27). This "catalyses" PE heating by improving the PE heating efficiency, allowing photons with lower energy to take part in the PE effect. This effect is the most significant at low  $\tau_B$ . In the following figures, I show the results for  $0.8 \le \tau_B \le 2.4$ , where valid solutions exist for all 4 example CR ionisation rates. At  $\tau_B = 0.8$ , the PE heating rate per H for  $\zeta_p = 1 \times 10^{-15} \text{ s}^{-1}$  is higher than the heating rate without CRs by 43%. To my knowledge, this effect has never been quantitatively investigated before.



FIGURE 3.25: PE heating rate in different CR ionisation rates, for  $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ 



FIGURE 3.26: Average electric charge of PAH grains (a = 5 Å) for  $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{\text{ini}} = 1$ 



FIGURE 3.27: Average electric charge of silicate grains (a = 10 Å) for  $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{\text{ini}} = 1$ 

Figure 3.28 shows the fraction of gas heating coming from CRs. This fraction can be thought of as the fraction of line emission that is "powered" by CRs. Increasing the CR ionisation rate has a significant effect in raising the fraction of gas heating from CRs.



FIGURE 3.28: Fraction of gas heating from CR heating as a function of  $\tau_{\rm B}$  and CR ionisation rate, for  $P_{\rm therm}/k_{\rm B} = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ 

#### 3.14.3 Influencing the gas chemistry

As described in Section 3.14.1, the extra electrons produced by CR ionisation shifts the C–C<sup>+</sup> balance towards C (recombination is favoured). This is clearly shown in Figure 3.29. For  $\zeta_p = 1 \times 10^{-15} \text{ s}^{-1}$ , the high gas temperature at  $\tau_B > 1.7$  causes the rising rate of  $n_C/n_{C^+}$  to decrease as the recombination rate of C<sup>+</sup> is extremely sensitive to gas temperature (see the  $k_{10}$  coefficient in Appendix B).



FIGURE 3.29: C/C<sup>+</sup> ratio as a function of  $\tau_{\rm B}$  and CR ionisation rate, for  $P_{\rm therm}/k_{\rm B} = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ 

Apart from changing the C/C<sup>+</sup> ratio, CR ionisation decreases the CO abundance since the formation of CO requires C<sup>+</sup> in my model. In addition, an increase in gas temperature decreases the rate of the C<sup>+</sup> + H<sub>2</sub>  $\longrightarrow$  CH<sub>2</sub><sup>+</sup> reaction (see Appendix B). Figure 3.30 illustrates the suppression of CO abundance due to CR ionisation. This has an effect of lowering the CO (1–0) emissivity per H, as Figure 3.31 shows. While the effect requires ~100 times CR fluxes at the solar circle to be present, it could potentially affect inferences of CR flux near CR sources. For example, if a cloud upstream of a supernova remnant shock became irradiated by CRs accelerated at the shock, the CO line would be depressed; and if the effect was not modelled, the CR flux would be underestimated.



FIGURE 3.30: CO abundance as a function of  $\tau_B$  and CR ionisation rate, for  $P_{therm}/k_B = 5 \times 10^3$  K cm<sup>-3</sup>,  $G_{ini} = 1$ 



FIGURE 3.31: CO(1–0) emissivity as a function of  $\tau_B$  and CR ionisation rate, for  $P_{\text{therm}}/k_B = 5 \times 10^3 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ 

# 3.14.4 Catalyst effect for $P_{\text{therm}}/k_{\text{B}} = 2 \times 10^4 \text{ K cm}^{-3}$ , $G_{\text{ini}} = 3$

The catalyst effect can be more clearly seen in at a thermal pressure of  $P_{\text{therm}}/k_{\text{B}} = 2 \times 10^4 \text{ K cm}^{-3}$ , when the pressure is large enough to allow the run with  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$  to have a valid solution. Figure 3.32 shows that at  $\tau_{\text{B}} = 0.6$ , the PE heating rate per H for  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$  is 45% higher than the run without CRs.



FIGURE 3.32: PE heating rate in different CR ionisation rates, for  $P_{\rm therm}/k_{\rm B} = 2 \times 10^4$  K cm<sup>-3</sup>,  $G_{\rm ini} = 3$ 

As shown in Figure 3.33, for  $\zeta_p = 3 \times 10^{-15} \text{ s}^{-1}$ , the fraction of gas heating from CR ionisation approaches 1 for  $\tau_B > 2$ . This implies that there may not be a link between the intensity of the UV-optical radiation field and the intensity of emission lines in highly obscured regions in the ISM (e.g. in dense molecular clouds). Rather, the strength of the emission lines in these regions may be tied to the CR flux and the gas chemistry.



FIGURE 3.33: Fraction of gas heating from CR ionisation for  $P_{\rm therm}/k_{\rm B}=2\times10^4~{\rm K~cm^{-3}},~G_{\rm ini}=3$ 

# 3.15 Comparison using different formulations of PE heating

Figure 3.34 shows a comparison of the gas temperature under different PE formulations of PE heating: the full PE calculation with the calculation of grain charging following Weingartner and Draine (2001b), and the analytic approximation given in Bakes and Tielens (1994). For low optical depths, the full PE calculation gives a significantly high gas temperature, indicating a higher PE heating rate. This is because the Weingartner and Draine (2001a) grain model contains a population of small dust grains (a < 50 Å), which is missing in the MRN grain model used in Bakes and Tielens (1994).



FIGURE 3.34: Comparing the gas temperature under different PE formulations of PE heating

# 3.16 Comparison of chemical model with model of Wolfire et al. (1995)

Wolfire et al. (1995) (Wolfire+95) introduced a thermal model for the diffuse ISM. Although the model takes the PE heating on dust grains from FUV photons and gas heating from X-rays into account, the gas heating is still dominated by the PE heating on dust grains. Figure 3.35 shows the comparison of gas density of my model with Wolfire+95, in which the data was taken from Figure 7 in Wolfire+95. To make a fair comparison, I used the values of helium abundance, gas-phase carbon and oxygen abundance and CR ionisation rate as used in Wolfire+95. Since Wolfire+95 uses the formulation of PE heating in Bakes and Tielens (1994) and the Draine (1978) ISRF, I use them as well.



FIGURE 3.35: Comparing the gas density with Wolfire et al. (1995) model. Following Wolfire et al. (1995), the PE heating formulation described in Bakes and Tielens (1994) is used

The results show good agreement between my model and Wolfire+95 for the range of thermal pressure compared. For  $P_{\text{therm}}/k_{\text{B}} > 4000 \text{ cm}^{-3}$ , Wolfire+95 gave a lower gas density (thus higher gas temperature). This is because of the inclusion of heating by photoionisation of C I in Wolfire+95, which is absent in my model. For  $P_{\text{therm}}/k_{\text{B}} < 4000 \text{ cm}^{-3}$ , Wolfire+95 gave a lower gas temperature because they considered the collisions between C II and electrons as well when they calculated the gas cooling rate due to the C II 158-µm fine-structure transition.

For 400 K cm<sup>-3</sup>  $< P_{\text{therm}}/k_{\text{B}} < 1600$  K cm<sup>-3</sup>, Wolfire+95 actually also gave three solutions (two stable and one unstable) for the gas density, where the lowest density

stable solution ( $n < 0.3 \text{ cm}^{-3}$ ) corresponds to the warm neutral medium. However, only the highest density (stable) solution is shown here, as my model is catered to finding solutions for the diffuse clouds and molecular clouds in the cold neutral medium.

# Chapter 4

# Augmented model with cosmic ray pressure and magnetic pressure

# 4.1 The insufficiency of thermal pressure

As turbulence, magnetic fields and cosmic rays permeate the ISM in galaxies, the pressure in the ISM has forms other than the thermal pressure: magnetic pressure, turbulent pressure and cosmic ray pressure. In the local part of the Milky Way, thermal pressure is only a minor portion ( $\sim$ 15%) of the total pressure (Jenkins and Tripp (2021)), which, in the Galactic midplane, is balanced against the weight of material in the gravitational potential of the Galactic plane (see, e.g. Boulares and Cox (1990)). Hence, in order to use the actual external pressure as the input of the ISM model developed in Chapter 3, it is important to also take the other pressure terms into account. In this chapter, the input pressure is expanded to encompass the CR pressure and magnetic pressure as well. The following shows a quick comparison of the different pressure terms under the typical conditions in the CNM:

1. Thermal pressure:

For an interstellar cloud in the CNM,

$$P_{\text{therm}} = nk_{\text{B}}T \approx 0.4 \text{ eV cm}^{-3} \left(\frac{n}{50 \text{ cm}^{-3}}\right) \left(\frac{T}{100 \text{ K}}\right).$$
 (4.1)

2. Cosmic ray pressure:

Using the CR spectra observed by *Voyager I* just outside the heliosphere (after correcting for solar modulation), the CR energy density  $\epsilon_{CR} \approx 1.0 \text{ eV cm}^{-3}$  (Cummings et al. (2016)).  $P_{CR} = \epsilon_{CR}/3$  in the relativistic case and  $P_{CR} = 2\epsilon_{CR}/3$  in the non-relativistic case. Therefore, the CR pressure  $P_{CR}$  satisfies 0.3 eV cm<sup>-3</sup>  $\leq P_{CR} \leq 0.6 \text{ eV cm}^{-3}$ . This will be explored further in Section 4.2.2.

### 3. Magnetic pressure

The magnetic pressure is 1/3 times the energy density of the magnetic field:

$$P_{\rm mag} = \frac{u_{\rm mag}}{3} = \frac{1}{3} \left( \frac{B^2}{8\pi} \right) \tag{4.2}$$

$$\approx 0.3 \,\mathrm{eV} \,\mathrm{cm}^{-3} \,\left(\frac{B}{6\,\mu\mathrm{G}}\right)^2.$$
 (4.3)

This shows that the magnetic pressure is of the same order of magnitude as the thermal pressure for diffuse clouds in the solar vicinity. In fact, analysis of measurements of magnetic field in interstellar clouds by Crutcher et al. (2010) shows that  $B \sim n^{0.65}$  for  $n \geq 300$  cm<sup>-3</sup>, so  $P_{\text{mag}} \sim n^{1.3}$ , whereas  $P_{\text{therm}} \sim n$  (assuming the gas temperature is constant). Therefore, for molecular clouds, the magnetic pressure grows faster than the thermal pressure with density. Thus, empirically, magnetic support is expected to be important in the central regions of self-gravitating clouds.

4. Turbulent pressure

Turbulent motions exist in various phases of the ISM on a wide range of spatial scales (see, e.g. the review by Elmegreen and Scalo (2004)). Turbulent pressure can be expressed as:

$$P_{\rm turb} = \rho \sigma_v^2 \tag{4.4}$$

where  $\rho$  is the mass density of the gas and  $\sigma_v$  is the internal velocity dispersion of the cloud. From the empirical data of a homogeneous sample of molecular clouds, Bonazzola et al. (1987) derived

$$\sigma_v \approx 0.4 \,\mathrm{km}\,\mathrm{s}^{-1} \left(\frac{R}{1\,\mathrm{pc}}\right)^{0.5}.\tag{4.5}$$

where *R* is the radius of the molecular cloud. From these relations, the turbulent pressure of a cloud is approximately

$$P_{\rm turb} \approx 0.2 \, \rm eV \, cm^{-3} \, \left(\frac{n_{\rm H}}{100 \, \rm cm^{-3}}\right) \left(\frac{R}{1 \, \rm pc}\right). \tag{4.6}$$

This shows that the turbulent pressure of a molecular cloud with size  $\gtrsim 1$  pc is at least comparable to the magnetic pressure. Physically, the turbulent pressure originates from bulk motions of gas with a thermodynamic pressure (i.e. as linked to temperature and density via an equation of state) which has no explicit relation to turbulent pressure. Since my model only addresses thermodynamic pressure, no term is included for  $P_{\text{turb}}$  in the total input pressure. Such a term does, however, need to be included when considering macroscopic properties of clouds (see Chapter 5).

# 4.2 Finding the cosmic ray pressure

### 4.2.1 Calculating cosmic ray ionisation rate from cosmic ray spectrum

Since *Voyager I* crossed the heliopause in August 2012, it has been observing the local interstellar energy spectra of Galactic cosmic-ray nuclei. Its observations of CR spectra and the fitting results of CR propagation models were described in Cummings et al. (2016). The GALPROP DR (Diffusive-reacceleration) model has the best fit to the *Voyager I* observations and its fitting data were chosen to be the standard CR spectra for protons and helium nuclei in the local ISM in this thesis (Table 13 in Cummings et al. (2016)).

The primary ionisation rate of atomic hydrogen in the interstellar medium due to species *i* in CRs (in  $s^{-1}$ ) is calculated by:

$$\zeta_{\mathrm{p},i} = 4\pi \int_{E_{\mathrm{low},i}}^{E_{\mathrm{high},i}} J_i(E)\sigma_i(E) \,\mathrm{d}E \tag{4.7}$$

where  $J_i(E)$  is the differential particle flux of species *i* in

particles cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> (GeV/nuc)<sup>-1</sup>,  $\sigma_i(E)$  is the ionisation cross-section of species *i* in cm<sup>2</sup>, *E* is the kinetic energy of the CR particle in GeV/nuc (GeV per nucleon). Figure 4.1 shows the empirically measured energy spectra of CR protons and helium nuclei as shown in Cummings et al. (2016).  $E_{low}$ , the lower bound of CR energy in the GALPROP DR model, is 3 MeV for CR protons and electrons and 3 MeV/nuc for cosmic ray helium nuclei.  $E_{high,p} = 1.07 \times 10^6$  GeV,  $E_{high,He} = 1.07 \times 10^6$  GeV/nuc and  $E_{high,e} = 1 \times 10^3$  GeV. For simplicity, for the calculation of the primary CR ionisation rate, only the ionisations due to CR protons, electrons and helium nuclei are considered. Note that in this work I describe these particles as "primary". In fact, as energy decreases, an increasing fraction may be secondary products of interactions of higher energy CR particles with the ISM.



FIGURE 4.1: Standard differential energy spectra for CR protons, He nuclei and electrons used in this work

The energy spectrum of CR electrons  $J_e(E)$  is taken from the analysis of *PAMELA* data by Potgieter et al. (2015), which is referred to as a Galactic electron spectrum (or more specifically a "very local interstellar spectrum" (LIS)):

$$J_{\rm e}(E) = J_{\rm LIS}(E) = 0.21 \left(\frac{E^{-1.35}}{\beta^2}\right) \left[\frac{E^{1.65} + 0.6920}{1.6920}\right]^{-1.1515}$$
(4.8)

where *E* is the kinetic energy of the CR electrons in GeV and  $J_e$  is in particles m<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> MeV<sup>-1</sup>. The  $J_{bump}$  term in Potgieter et al. (2015) is excluded, since the inclusion of the term would make the energy density of CR electrons much higher than what was calculated in Cummings et al. (2016). This energy spectrum, of course, relates to the local CR electrons in the ISM.

The ionisation cross section  $\sigma(E)$  can be calculated as follows. Considering that the target particle is a hydrogen atom, the collisional ionisation cross-section of particles with charge *Ze* and velocity  $\beta c$  is given by (Bethe (1933))

$$\sigma(Z,\beta) = 0.285 \frac{2\pi e^4 Z^2}{m_e c^2 I_H \beta^2} \left( \ln \left[ \frac{2m_e c^2 \beta^2}{I_H (1-\beta^2)} \right] + 3.04 - \beta^2 \right)$$
(4.9)

for  $\beta \gtrsim 0.025$ .  $I_{\rm H} = 13.6$  eV is the ionisation potential of atomic hydrogen. This equation can be evaluated to obtain (Cummings et al. (2016))

$$\sigma(E,Z) = 1.23 \times 10^{-20} \,\mathrm{cm}^2 \left(\frac{Z^2}{\beta^2}\right) \left(6.20 + 2\log(\gamma_{\mathrm{rel}}\beta) - 0.43\beta^2\right),\tag{4.10}$$

where  $\beta = v/c$ ,  $E = (\gamma_{rel} - 1)mc^2$  is the kinetic energy of the energetic particle and  $\gamma_{rel} = (1 - \beta^2)^{-1/2}$ . The ionisation cross-section of hydrogen atoms by CR protons, helium nuclei and electrons are shown in Figure 4.2.



FIGURE 4.2: Cross sections of the ionisation of hydrogen atoms by CR protons, helium nuclei and electrons, calculated using Equation 4.10

Usually the formulae above, the primary CR ionisation rate of atomic hydrogen due to CR protons, electrons and helium nuclei individually can be found. The total primary CR ionisation rate of atomic hydrogen, based on these CR spectra, is

$$\zeta_{\rm p} = \zeta_{\rm p,p} + \zeta_{\rm p,He} + \zeta_{\rm p,e} \tag{4.11}$$

$$= 5.04 \times 10^{-18} \,\mathrm{s}^{-1} + 1.59 \times 10^{-18} \,\mathrm{s}^{-1} + 1.51 \times 10^{-18} \,\mathrm{s}^{-1} \tag{4.12}$$

$$= 8.15 \times 10^{-18} \,\mathrm{s}^{-1}. \tag{4.13}$$

It is assumed that the CR spectra has the same shape in different environments, namely in the interstellar clouds in the Milky Way and in external galaxies.

However, does the calculated primary CR ionisation rate increase if  $E_{low}$  is lower than 3 MeV/nuc? Figure 4.3 shows the variation of primary CR ionisation rate due

to CR protons with  $E_{\text{low}}$ , assuming that J(E) of CR protons with E < 3 MeV is the same as J(E) at E = 3 MeV (particle flux = 1.4 particles cm<sup>-2</sup> s<sup>-1</sup> sr<sup>-1</sup> GeV<sup>-1</sup>). The results show that primary CR ionisation rate does increase with decreasing  $E_{\text{low}}$  and it approaches  $7 \times 10^{-18}$  s<sup>-1</sup> as  $E_{\text{low}}$  approaches 13.6 eV. However, since empirical measurements of CR spectra below E = 3 MeV is not available, the value obtained in Equation 4.13 is used in this work as the primary CR ionisation rate due to the CR spectra in Figure 4.1.



FIGURE 4.3: Variation of primary CR ionisation rate by CR protons with  $E_{low}$ , assuming that J(E) of CR protons with E < 3 MeV is the same as J(E) at E = 3 MeV.

### 4.2.2 Cosmic ray pressure

Using  $P = \epsilon/3$  (pressure is 1/3 of the energy density, as in photons), the pressure due to species *i* in CRs is given by (Cummings et al. (2016)):

$$P_{\text{CR},i} = \frac{4\pi N_i}{3} \int_{E_{\text{low},i}}^{E_{\text{high},i}} \frac{J_i(E) \cdot E}{v_i(E)} \, \mathrm{d}E \tag{4.14}$$

where  $N_i$  is the number of nucleons of the CR particle and  $v_i(E)$  is the velocity of the CR particle. The total CR pressure is the sum of the pressure components from CR

protons, helium nuclei and electrons:

$$P_{CR} = P_{CR,p} + P_{CR,He} + P_{CR,e}$$

$$= 3.82 \times 10^{-13} \text{ erg cm}^{-3} + 9.37 \times 10^{-14} \text{ erg cm}^{-3} + 1.98 \times 10^{-14} \text{ erg cm}^{-3}$$

$$(4.16)$$

$$= 4.95 \times 10^{-13} \text{ erg cm}^{-3} \tag{4.17}$$

$$= 3591 k_{\rm B} \,{\rm K} \,{\rm cm}^{-3} \approx 0.31 \,{\rm eV} \,{\rm cm}^{-3} \tag{4.18}$$

Therefore, a linear relationship between the primary CR ionisation rate and the total CR pressure can be found:

$$P_{\rm CR, \, tot} = 4406 \, k_{\rm B} \, {\rm K} \, {\rm cm}^{-3} \left( \frac{\zeta_{\rm p}}{10^{-17} \, {\rm s}^{-1}} \right)$$
(4.19)

$$\approx 0.38 \text{ eV cm}^{-3} \left( \frac{\zeta_{\rm p}}{10^{-17} \, {\rm s}^{-1}} \right)$$
 (4.20)

As the slope for E < 100 MeV/nuc in Figure 4.1 becomes flat, it is assumed that CR particles with energy below 3 MeV/nuc have negligible contribution to the total primary CR ionisation rate.

# 4.3 Interstellar magnetic fields

The relationship between the gas mass density  $\rho$  and magnetic field strength  $|\mathbf{B}|$  is usually stated in the form of a power law:  $|\mathbf{B}| \propto \rho^n$  (Crutcher (1999)). For a spherical cloud with radius *R* and total mass *M*, if the magnetic field is unimportant throughout the collapse of the cloud, the conservation of magnetic flux ( $\Phi_B = \pi R^2 |\mathbf{B}|$ ) implies  $|\mathbf{B}| \propto R^{-2}$ . On the other hand, conservation of mass ( $M = (4/3)\pi R^3 \rho$ ) suggests  $\rho^{2/3} \propto R^{-2}$ . Therefore, theory suggests that  $|\mathbf{B}| \propto \rho^{2/3}$ .

Observational studies of interstellar clouds yield results that are similar to the relation derived from theory. Crutcher et al. (2010) presented an analysis of Zeeman measurements of the magnitude of the line-of-sight component of the magnetic field  $|B_z|$  in diffuse clouds and molecular clouds (Figure 4.4). The solid black segments show the most probable model from the comprehensive analysis in Crutcher et al.'s paper. However, they seem to be too high for most data points. Therefore, the red line segments, which pass through the clusters of data points, are used in this thesis to predict  $|B_z|$  from  $n_{\rm H}$ :

$$|B_z| = \begin{cases} 3 \ \mu G, & n_{\rm H} \le 10^3 \ {\rm cm}^{-3} \\ 3 \ \mu G \left(\frac{n_{\rm H}}{10^3 \ {\rm cm}^{-3}}\right)^{0.765}, & n_{\rm H} > 10^3 \ {\rm cm}^{-3} \end{cases}$$
(4.21)



FIGURE 4.4: Strength of the line-of-sight component of the interstellar magnetic field versus  $n_{\rm H}$  in clouds. The red line is my function for predicting  $|B_z|$  from  $n_{\rm H}$ . The solid black line is the fitting function used in Crutcher et al. (2010). Figure modified from Crutcher et al. (2010).

Using the assumption that  $|\mathbf{B}| = 2|B_z|$  (assuming that the magnetic fields of clouds are randomly oriented), as used in Crutcher (1999) and Troland and Crutcher (2008), and using *B* as the shorthand for  $|\mathbf{B}|$ ,

$$B = \begin{cases} 6 \ \mu G, & n_{\rm H} \le 10^3 \ {\rm cm}^{-3} \\ 6 \ \mu G \left(\frac{n_{\rm H}}{10^3 \ {\rm cm}^{-3}}\right)^{0.765}, & n_{\rm H} > 10^3 \ {\rm cm}^{-3} \end{cases}$$
(4.22)

The magnetic pressure in clouds can then be easily found from the relation between magnetic energy density  $\epsilon_{mag}$  and *B*:

$$P_{\rm mag} = \frac{\epsilon_{\rm mag}}{3} = \frac{1}{3} \left(\frac{B^2}{8\pi}\right) = 4.77 \times 10^{-13} \,\rm erg \, cm^{-3} \, \left(\frac{B}{6 \,\mu\rm G}\right)^2 \tag{4.23}$$

$$= 3458 k_{\rm B} \,\mathrm{K} \,\mathrm{cm}^{-3} \,\left(\frac{B}{6\,\mu\mathrm{G}}\right)^2 \tag{4.24}$$

$$\approx 0.36 \text{ eV cm}^{-3} \left(\frac{B}{6\,\mu\text{G}}\right)^2 \tag{4.25}$$

# 4.4 Slab calculations

Since CR pressure and magnetic pressure are incorporated into the model, the total pressure  $P_{tot}$  becomes an input of the model:

$$P_{\rm tot} = P_{\rm therm} + P_{\rm CR} + P_{\rm mag} \tag{4.26}$$

The thermal pressure  $P_{\text{therm}}$  becomes an unknown quantity rather than an input of the model. In the loop finding  $n_{\text{H}}$ , it is insufficient to just use the ideal gas law with  $P_{\text{therm}}$ . Instead, I plug trial values of  $n_{\text{H}}$  into the right hand side of Equation 4.26 until the sum of the right hand side is equal to  $P_{\text{tot}}$ :

$$P_{\text{tot}} = P_{\text{therm}}(T, n_{\text{H}}, f_{\text{H}_2}) + P_{\text{CR}}(\zeta_{\text{p}}) + P_{\text{mag}}(n_{\text{H}})$$
(4.27)

The other loops remain the same. The effect of using this equation is that part of the total pressure is shared by the magnetic field and the CRs. Therefore, compared to the model without magnetic field, one needs a higher total pressure to obtain valid solutions for the same radiation field and CR ionisation rate. Basically, this is a new equation of state for the gas with the state function  $P_{\text{tot}}(T, n_{\text{H}}, f_{\text{H}_2})$ .

## **4.4.1 Run 1: low** $P_{\text{tot}}$ , **low** $G_{\text{ini}}$ and **low** $\zeta_{\text{p}}$

The following plots show the slab calculation when  $P_{\text{tot}} = 1 \times 10^5 k_{\text{B}}$  K cm<sup>-3</sup>,  $G_{\text{ini}} = 1$  and  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ . Overall, the results are qualitatively similar to the simple model of Chapter 3 with  $P_{\text{therm}}/k_{\text{B}} = 5 \times 10^3$  K cm<sup>-3</sup>, low external ISRF and low CR ionisation rate (Section 3.12.1). However, the gas temperatures is lower and the densities are higher due to low fraction of thermal pressure. This is just because a higher total pressure is used. From Figure 4.6 it can be seen that the thermal pressure decreases with increasing  $\tau_{\text{B}}$  (increasing  $n_{\text{H}}$ ), while the magnetic pressure increases with increasing  $n_{\text{H}}$  since  $P_{\text{mag}} \propto n_{\text{H}}^{1.53}$ .



FIGURE 4.5: Temperature, molecular fraction, hydrogen density and electron density for  $P = 1 \times 10^5 k_B \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_p = 3 \times 10^{-17} \text{ s}^{-1}$ 



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 4.6: Pressure components for  $P_{\text{tot}} = 1 \times 10^5 k_{\text{B}} \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

Figure 4.7 shows the abundances of major species (except He I). Qualitatively, the gas composition for  $0 \le \tau_B \le 2$  resembles the low pressure, low ISRF and low CRIR run in Chapter 3 (Figure 3.9).



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 4.7: Abundances of major species (except He I) for  $P_{tot}/k_B = 1 \times 10^5$  K cm<sup>-3</sup>,  $G_{ini} = 1$ ,  $\zeta_p = 3 \times 10^{-17}$  s<sup>-1</sup>

Figure 4.8 shows the gas heating and cooling rates. Heating by gas-dust collisions surpasses PE heating at  $\tau_B \approx 1.8$  and dominate gas heating afterwards, while the cooling due to CI lines dominates gas cooling for  $1.3 \le \tau_B \le 2.3$ .



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17}$  s<sup>-1</sup>

FIGURE 4.8: Gas heating and cooling rates for  $P_{tot}/k_B = 1 \times 10^5$  K cm<sup>-3</sup>,  $G_{ini} = 1$ ,  $\zeta_p = 3 \times 10^{-17}$  s<sup>-1</sup>



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5$  K cm<sup>-3</sup>,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17}$  s<sup>-1</sup>

FIGURE 4.9: Gas heating rates for  $P_{\rm tot}/k_{\rm B}=1 imes10^5$  K cm<sup>-3</sup>,  $G_{\rm ini}=$  1,  $\zeta_{\rm p}=3 imes10^{-17}$  s<sup>-1</sup>



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 4.10: Line emissivities for  $P_{\rm tot}/k_{\rm B}=1\times10^5$  K cm<sup>-3</sup>,  $G_{\rm ini}=1, \zeta_{\rm p}=3\times10^{-17}$  s<sup>-1</sup>

Figure 4.11 shows the 5 CO rotational line emissivities per H. The crossing between the CO (1–0) line and the CO (3–2) line is because low *T* favours the CO (1–0) line more than the CO (3–2) line.



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^5 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 1$ ,  $\zeta_{\rm p} = 3 \times 10^{-17} \text{ s}^{-1}$ 

FIGURE 4.11: CO line emissivities for  $P_{\text{tot}}/k_{\text{B}} = 1 \times 10^5 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 1$ ,  $\zeta_{\text{p}} = 3 \times 10^{-17} \text{ s}^{-1}$ 

# **4.5 Run 2:** high $P_{\text{tot}}$ , high $G_{\text{ini}}$ and high $\zeta_p$

The following plots show the slab calculation when  $P_{\text{tot}}/k_{\text{B}} = 1 \times 10^7 k_{\text{B}}$  K cm<sup>-3</sup>,  $G_{\text{ini}} = 100$  and  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ . The conditions are similar to a PDR near a starforming region with high CR ionisation rate. Qualitatively, the behaviours of *T*,  $n_{\text{H}}$  and molecular fraction resemble the high pressure run in Chapter 3 (see Figure 3.14). The abundances of major species (Figure 4.14) also show a remarkable resemblance to Figure 3.16. At  $\tau_{\text{B}} \simeq 3$ , the abundances of C<sup>+</sup>, C and CO are also very close to each other.



FIGURE 4.12: Temperatures, molecular fraction, hydrogen density and electron density for  $P_{\text{tot}}/k_{\text{B}} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\text{ini}} = 100$ ,  $\zeta_{\text{p}} = 3 \times 10^{-15} \text{ s}^{-1}$ 

Figure 4.13 shows the composition of the total pressure. Note that the magnetic pressure dominates the pressure in the slab for  $\tau_{\rm B} > 0.4$ .


FIGURE 4.13: Pressure components for  $P_{tot} = 1 \times 10^7 k_B \text{ K cm}^{-3}$ ,  $G_{ini} = 100$ ,  $\zeta_p = 3 \times 10^{-15} \text{ s}^{-1}$ 

Figure 4.14 shows the abundances of the major species in the gas (except He I). This is qualitatively similar to Figure 3.16.



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 4.14: Abundances of major species (except He I) for  $P_{\rm tot}/k_{\rm B}=1\times10^7$  K cm<sup>-3</sup>,  $G_{\rm ini}=100$ ,  $\zeta_{\rm p}=3\times10^{-15}$  s<sup>-1</sup>

Figure 4.15 shows the heating and cooling rate for this run. PE heating transitions into CR heating at approximately the same optical depth as C II cooling transitions into CO cooling ( $\tau_B \approx 2.8$ ).



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 4.15: Gas heating and cooling rates for  $P_{tot}/k_B=1\times 10^7$  K cm<sup>-3</sup>,  $G_{ini}=100$ ,  $\zeta_p=3\times 10^{-15}$  s<sup>-1</sup>



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 4.16: Gas heating rates for  $P_{tot}/k_B = 1 \times 10^7$  K cm<sup>-3</sup>,  $G_{ini} = 100$ ,  $\zeta_p = 3 \times 10^{-15}$  s<sup>-1</sup>

Figure 4.17 shows the line emissivities per H. As  $\tau_B$  increases, line emission is dominated by the [O I] 63 µm line, the [C II] 158 µm line, then the CO rotational lines (see Figure 4.18).



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 4.17: Line emissivities for  $P_{tot}/k_B = 1 \times 10^7$  K cm<sup>-3</sup>,  $G_{ini} = 100$ ,  $\zeta_p = 3 \times 10^{-15}$  s<sup>-1</sup>



 $P_{\rm tot}/k_{\rm B} = 1 \times 10^7 \text{ K cm}^{-3}$ ,  $G_{\rm ini} = 100$ ,  $\zeta_{\rm p} = 3 \times 10^{-15} \text{ s}^{-1}$ 

FIGURE 4.18: Line emissivities for  $P_{tot}/k_B = 1 \times 10^7$  K cm<sup>-3</sup>,  $G_{ini} = 100$ ,  $\zeta_p = 3 \times 10^{-15}$  s<sup>-1</sup>

# 4.6 Comparing with the model in Chapter 3

The figures so far did not quantitatively demonstrate the effect of the different pressure formulation. The following figures show the comparison of this model with the simpler model in Chapter 3, using the same thermal pressure at  $\tau_{\rm B} = 0$  in Run 1 in this chapter ( $P_{\rm therm}/k_{\rm B} = 6.13 \times 10^4$  K cm<sup>-3</sup>). The results are very similar for the variation of the gas temperature with  $\tau_{\rm B}$ . As  $\tau_{\rm B}$  increases, there is a less strong increase in density so gas cooling is suppressed. However, in PE dominated heating, the heating goes as  $\sim n^2$ . So the cooling and heating are balanced as before.

In the Chapter 3 model (the model without magnetic field), the thermal pressure is kept at a constant value, whereas the thermal pressure in the model with magnetic field decreases with  $\tau_{\rm B}$  according to Figure 4.6. This means that  $n_{\rm H}$  obtained from the model with magnetic field is lower than that obtained from the model without magnetic field, as shown in Figure 4.20. As  $\tau_{\rm B}$  increases, an increasing part of the thermal pressure at  $\tau_{\rm B} = 0$  changes into magnetic pressure.



FIGURE 4.19: Comparing the gas temperature output of the model in this chapter (with magnetic field) and the model in Chapter 3 (without magnetic field). The orange line is exactly the same as the gas temperature line in the top left plot in Figure 4.5. The inputs in the title of this plot applies to the model without magnetic field.



FIGURE 4.20: Comparing the output of  $n_{\rm H}$  from the model in this chapter (with magnetic field) and the model in Chapter 3 (without magnetic field). The orange line is exactly the same as the top right plot in Figure 4.5. The inputs in the title of this plot applies to the model without magnetic field.

Self-gravitating clouds of a given mass will have a lower gas density if they have magnetic fields. This means that they will have a lower optical depth, provided that the interior density exceeds  $\sim 1000 \text{ cm}^{-3}$ . Clouds with magnetic fields and cosmic ray flux are more transparent, so PE heating dominates further into the cloud. It also follows that the change to CR-dominated heating (e.g. as explored in Chapter 3) will occur deeper in magnetised clouds. This shows that the radiation field, magnetic field and cosmic rays all play a role in the density structure of interstellar clouds.

In real astrophysical systems, we may also expect a variation of  $\zeta_p$  with density - e.g. in magnetised clouds, we might expect systematic variation of  $\zeta_p$  with  $n_H$  and B. These effects would require self-consistent solutions of the CR transport equation. This is well beyond the scope of this dissertation.

# Chapter 5

# Application to cloud models

# 5.1 Introduction

Having built a model of simple chemistry and thermal physics of the neutral and molecular ISM, it is time to apply the model to gas in the ISM with real radiation fields. Under typical conditions, gas in molecular form can only exist when radiation fields are attenuated by dust, and/or the ambient pressure is enhanced. Both these trends happen in clouds, where the ambient ISRF is attenuated by dust, and the ambient pressure is increased, due to the balance between pressure support and gravitational potential.

As a first application, the model is used to calculate the PE heating of gas in the clouds in the nearby spiral galaxy NGC 628. This galaxy has detailed observations of individual molecular clouds measured in the CO lines by ALMA (see. e.g. Herrera et al. (2020)), and moreover has global solutions for the diffuse UV-optical-NIR (near infrared) ISRF throughout the galaxy. The UV-to-submillimetre (sub-mm) ISRF of NGC 628 have been obtained using a self-consistent axisymmetric radiative transfer (RT) code described in Popescu et al. (2011) to model the direct and dust-reradiated starlight throughout the galaxy (Rushton et al. (2022)). This allows the external ISRF incident on clouds to be known. In this chapter I introduce a simple spherically symmetric model for self-gravitating clouds, which predicts line emission from these clouds as a function of the external ISRF on the cloud, the ambient pressure of the ISM in which the cloud is situated, and the mass of the cloud. We then compare model predictions with observations of CO line emission in the ISM of NGC 628.

## 5.1.1 "Passive" and "Active" clouds

For the purposes of analysing dust emission from star-forming galaxies, it is important to classify interstellar clouds into "passive" and "active" clouds, as discussed in Popescu et al. (2011). "Active" clouds, or "birthclouds" as referred to in Popescu et al. (2011), are clouds that are actively forming stars. The dust and gas in the cloud are strongly heated, predominantly by UV light emitted by young massive stars in close proximity to the clouds. As a consequence, the clouds emit warm dust emission (SED peaks in the 25-100  $\mu$ m range). In addition, in case of strong gas heating, such clouds are preferentially detected as individual objects in flux-limited CO line surveys. "Passive" clouds, on the other hand, are not actively forming stars and are relatively far from star-forming regions. They do not have internal sources of starlight, and their dust and gas are heated by the diffuse ISRF. They predominantly emit cold dust emission (SED peaks in the 100-200  $\mu$ m range). Since the dust emission SEDs of spiral galaxies peak in the 100-200  $\mu$ m range, most gas in spiral galaxies is not associated with star-forming regions, instead existing either in "passive" clouds or in an extended diffuse medium. For the purposes of modelling interstellar clouds heated by the diffuse ISRF with RT codes, it is important to make sure the clouds are passive so that they do not have internal sources of starlight. Because only then can we be confident that the radiation field illuminating the external boundary of the cloud is indeed the diffuse ISRF as modelled from large-scale RT calculations of a galaxy.

# 5.2 Observations

### 5.2.1 Observational data for NGC 628

NGC 628 is a large, star-forming, late-type spiral galaxy (Honig and Reid, 2015) that is nearly face-on and nearby (distance =  $9.52^{+0.26}_{-0.41}$  Mpc (Scheuermann et al. (2022))). Due to its properties, it is ideal for studies on a variety of topics (Rushton et al. (2022)), including galaxy evolution and stellar populations (e.g. Natali, Pedichini, and Righini (1992)), star formation (e.g. Hodge (1976)), interstellar medium (e.g. Berg et al. (2013)), and galaxy dynamics (e.g. Honig and Reid, 2015). Figure 5.1 shows the images of NGC 628 from ALMA CO (2–1) (Leroy et al. (2021)) and JWST MIRI 21 µm (Leroy et al. (2023)) at the same angular resolution before processing. A large component of the JWST 21 µm emission likely originates from warm dust heated by UV emission from star-forming (active) clouds. With this in mind, it appears that the CO line emission and star-forming clouds have similar spatial distributions in NGC 628. Referring to the emission properties of active clouds in Section 5.1.1, we use high angular resolution JWST measurements for 21-µm emission as a tracer for active clouds.



FIGURE 5.1: Images of NGC 628 at the same angular resolution. ALMA CO (2–1) (Leroy et al. (2021)) (left) and JWST-MIRI 21  $\mu m$  (Leroy et al. (2023)) (right)

Nevertheless, there is also evidence for passive molecular clouds in NGC 628. In particular, Chevance et al. (2020) quantified the evolutionary timeline of giant molecular clouds (GMCs) in nearby star-forming disc galaxies including NGC 628. They estimated that CO emission was visible from GMCs in NGC 628 from ~24 Myr ago to 3 Myr ago, while neither H  $\alpha$  emission, nor, for almost all this time, 21  $\mu$ m emission from birthclouds, were visible in that period. As H  $\alpha$  emission requires ionising radiation from the formation of massive stars, this indicates that GMCs experience a long inert phase (75–90 percent of cloud lifetime (Chevance et al. (2020))) in which they are passive, before the emergence of massive stars. This indicates the existence of passive clouds in disc galaxies.

Figure 5.2 shows the H I 21 cm, 4.5  $\mu$ m and 500  $\mu$ m and CO (2–1) line emission observations of NGC 628, which were obtained from different instruments.



FIGURE 5.2: Azimuthally averaged profiles of flux per beam of the H I 21 cm line, velocity-integrated line intensity of the CO (2–1) line, flux per unit frequency interval at 4.5  $\mu$ m and 500  $\mu$ m of NGC 628 as a function of galactocentric radius. 1 MJy =  $10^{-17}$  erg cm<sup>-2</sup> s<sup>-1</sup> Hz<sup>-1</sup>. Data sources: H I 21 cm – THINGS (Walter et al. (2008)), CO (2–1) – HERACLES (Leroy et al. (2009)), 4.5  $\mu$ m – *Spitzer*-IRAC (Fazio et al. (2004)), 500  $\mu$ m – KINGFISH with *Herschel* (Kennicutt et al. (2011))

#### 5.2.2 Measuring CO line emission from passive clouds in NGC 628

Thanks to the sub-arcsecond angular resolution of ALMA and JWST, these facilities enable detection and measurements of individual clouds even in galaxies at a distance of 9.5 Mpc as is the case for NGC 628. This, in turn allowed active clouds to be selected at 21  $\mu$ m from the JWST maps, and their CO (2–1) flux to be measured from the ALMA maps. Results are shown in Figure 5.3. There is a broad correlation, which we used to fix an empirical relation between the 21- $\mu$ m flux and CO (2–1) line flux for active clouds. Our strategy was to use this relation to remove the component of CO (2–1) emission associated with active clouds from images of CO (2–1) in NGC 628, thus providing radial profiles of CO (2–1) emission from passive clouds.



FIGURE 5.3: Correlation between JWST 21- $\mu$ m line flux density and the PHANGS-ALMA CO (2–1) velocity-integrated line brightness for individual active clouds selected at 21  $\mu$ m on the JWST images. Photometry was performed on high-pass Fourier-filtered ALMA (Leroy et al. (2021)) and JWST (Leroy et al. (2023)) images. The colour coding relates to the position of a cloud in the galaxy (blue = large galactocentric radius, yellow = small galactocentric radius).

Unfortunately, the sensitivity of ALMA is limited to relatively bright clouds in the CO line. Moreover, interferometers may resolve out emission from an ensemble of parent clouds. For that reason, to measure passive clouds which may be faint, one has to utilise single dish image, which we did using the HERACLES image of NGC 628 in the CO (2–1) line.

To create a spatial photometric template of warm dust tracing birthclouds in NGC 628, we also needed to subtract mid-infrared continuum light from transiently heated grains in the diffuse ISM, for which we used the RT models of Rushton et al. (2022). Specifically, this is subtracted from the 24  $\mu$ m *Spitzer*/MIPS image of NGC 628<sup>-1</sup>. This yields a "pure" image of the brightness due to all active clouds in NGC 628. We multiplied the image by the scaling factor CO (2–1)/21  $\mu$ m derived from Figure 5.3 to create a corresponding image of CO (2–1) emission from active clouds, shown in Figure 5.4.

<sup>&</sup>lt;sup>1</sup>The MIPS image has much better surface brightness, sensitivity and photometric precision than the JWST 21  $\mu$ m, so it was used to create the photometric template for active clouds



FIGURE 5.4: Azimuthally averaged profile of the 24-µm brightness using observational data from *Spitzer*/MIPS (Rieke et al. (2004))

Finally, we subtracted the image of CO (2–1) emission from active clouds from the HERACLES image of CO (2–1) to create an image of CO (2–1) from passive clouds as shown in Figure 5.5. One sees that the CO emission not associated with warm dust dominates. This is consistent with a large population of CO-emitting clouds with low ratios of CO-to-warm dust emission, which we identify with passive clouds.



FIGURE 5.5: Azimuthally averaged profile of velocity-integrated CO (2–1) line intensity in NGC 628, using observational data from HER-ACLES (Leroy et al. (2009))



### 5.2.3 Deriving the radiation field, total pressure, gas and dust content

FIGURE 5.6: Azimuthally averaged profiles of the radiation field, total pressure, gas surface density and dust surface density in the midplane of NGC 628 as a function of galactocentric radius. These quantities are derived by the RT model.

The top left panel in Figure 5.6 shows the energy densities of the UV-visible radiation field in the midplane of NGC 628, separated into the three bands defined in Section 2.5.1. These energy densities are the solutions of the RT code described in Popescu et al. (2011) as found by Rushton et al. (2022). The pressure in the top right panel is the total pressure in the galactic disc of NGC 628 resulting from gravitational potential (see Appendix **G** for the full derivation).

# 5.3 A simple semi-analytical spherical cloud model

### 5.3.1 Introduction and input parameters

Since the mass distribution of clouds in NGC 628 cannot be directly known from observations, a simple semi-analytical cloud model for spherically symmetric homogeneous clouds, developed by Richard Tuffs and loosely based on models by van Dishoeck and Black (1986), was used to simulate spherical clouds of different masses in the galaxy. While very simple, this model has a single parameter  $M_{cloud}$  (cloud mass) for a cloud in a region of known external ISRF and known pressure, with no internal sources of starlight. This makes it possible to provide a relatively simple comparison of predicted and observed surface brightness of CO line from those ensemble of passive clouds in the galaxy.

The cloud model solves for the scale radius  $r_{\text{scale}}$ , truncation radius  $r_{\text{trunc}}$ , internal illumination and pressure of virially supported passive spherical clouds of gas and dust, following the semi-analytic treatment described in Appendix **F**. The output quantities listed above are expressed as a function of the external diffuse ISRF, pressure and metallicity of the ISM at the galactocentric radii where the clouds are situated, as can be derived from RT modelling of the large scale propagation of direct and dust-reradiated starlight in galaxies.

The model adopts a fixed radial distribution of density according to a King profile, which is an approximate solution of the equation of hydrostatic support of an isothermal self-gravitating cloud (see Equation 5.2). For low mass clouds (up to a few solar masses, which are transparent to an external radiation field heating the cloud), pressure can be provided entirely by the thermal pressure of the gas. But for more massive clouds, which become optically thick, this is no longer the case, because when the illumination drops, balance of heating and cooling requires higher densities and lower temperatures. In essence, this means that massive passive clouds assuming this fixed density structure must be inhomogeneous and the density profile can only be maintained by bulk motion of denser substructure.

As such, any homogeneous model of a massive cloud is unphysical. However, such a homogeneous model can nevertheless provide a robust check on the hypothesis that the heating of gas in passive clouds is due to PE heating powered by the external ISRF. It was also found that the model predicts the typical range of scales and densities of clouds observed in the ISM.

The input parameters to this model are:

- As a function of galactocentric radius:
  - ISRF from global RT model of Rushton et al. (2022)
  - external pressure from global RT model of Rushton et al. (2022)
  - metallicity from Berg et al. (2013)
- Independent of galactocentric radius:
  - dust model of Weingartner and Draine (2001a) with fraction of metals in grains  $F_{gr} = [0.7, 0.7]$
  - primary cosmic ray ionisation rate per H is set to  $3 \times 10^{-17}$  s<sup>-1</sup> (typical of clouds at the solar circle in the Milky Way). In principle this may vary, but we fix it here. It will be an underestimate.
  - velocity dispersion of 15 km s<sup>-1</sup> (derived from ALMA data)

#### 5.3.2 The treatment of turbulence

In the model, the cloud maintains its fixed radial profile through a virial support of bulk motions, which has long been known to be an important ingredient against gravitational collapse in molecular clouds (e.g. Larson (1981)). Since it is computationally difficult to model turbulence in different scales, as a simple approximation, turbulence in this simple model is treated as a component in the virial velocity  $v_{vir}$  of a cloud in hydrostatic equilibrium. For a cloud supported by just thermal pressure (e.g. Galactic cirrus clouds),

$$v_{\rm vir} = \sqrt{\frac{3k_{\rm B}T}{\mu m_{\rm H}}},\tag{5.1}$$

where  $\mu$  is the mean molecular weight of the gas and  $m_{\rm H}$  the mass of a hydrogen atom. For clouds supported by turbulent motion,  $v_{\rm vir} > \sqrt{3k_{\rm B}T/\mu m_{\rm H}}$ .

#### 5.3.3 Gas density profile in the cloud model

For the incorporation into an ISRF calculated by a large-scale RT code, each cloud in the cloud model can be thought of as a "pseudo-grain", which is parameterised as a spherically symmetrical truncated King profile. The King profile has a gas density profile of

$$\rho(r) = \rho_0 \left[ 1 + \left(\frac{r}{l}\right)^2 \right]^{-3/2}$$
(5.2)

for  $0 \le r \le r_{trunc}$ , where  $\rho_0$  is the density at r = 0, l is a scale length and  $r_{trunc}$  is a truncation radius.  $\rho_0$ , l and  $r_{trunc}$  are all internal parameters in this model. The model divides the whole cloud into a number of shells, and solves the B-band optical depth  $\tau_B$  from the outer radius of each shell to the surface of the cloud. An RT calculation is done in the optical/NUV/FUV continuum to measure the illumination of gas and dust in each shell of a cloud by the external ISRF. This illumination is then used as an input to the thermodynamic model to measure abundances of species such as CO and H<sub>2</sub>. The treatment also considers iteratively the effect on the transfer of FUV light by dissociation of H<sub>2</sub>, following the approximate treatment of Sternberg et al. (2014), as well as the effect of non-local absorption of CO line photons on the excitation of the CO molecule. RT calculations are performed in the CO line to predict the emergent CO line flux as a function of the mass of the cloud. It is this quantity that is the basis for the comparison with the measurements of CO line flux from the ensemble of passive clouds.

The RT calculations are done assuming a homogeneous distribution of gas in each shell. As mentioned, this is only realistic for low mass clouds. High mass molecular clouds are expected and observed to have a clumpy structure. However, the RT calculations made assuming homogeneity place an upper limit on the illumination of gas in the clouds and a lower limit on the opacity in the CO lines. As such, the calculations can be used to check the consistency of the hypothesis that PE heating by the diffuse ISRF is powering the CO line emission, as well as limits on the value of the  $X_{CO}$  factor relating H<sub>2</sub> column density to CO line brightness.

The external pressure at the surface of the cloud  $P_{\text{ext}}$  is an input parameter of the model, and it comes from the total pressure in the galactic disc as a function of the galactocentric radius and height above the galactic disc. It is taken as  $P_{\text{therm}}$  if the model in Chapter 3 is used, or taken as  $P_{\text{tot}}$  if the model in Chapter 4 is used. The outermost shell is always taken to be fully illuminated by the external radiation field. The pressure at the centre of the cloud,  $P_{\text{centre}}$ , is one of the outputs of the model, and can either be  $P_{\text{therm}}$  or  $P_{\text{tot}}$  depending on which pressure model is used.

Figure 5.7 is a schematic diagram showing the onion-like structure of a spherical cloud in the semi-analytical cloud model. The molecular gas in the core is too cold so there is hardly any CO line emission. CO emission is concentrated in a ring with slightly warmer  $H_2$  as the CO distribution in general follows the  $H_2$  distribution.



FIGURE 5.7: Schematic diagram showing the structure of a spherical cloud in the semi-analytical cloud model

The outputs of the model are

- ratio of truncation radius to cloud scale radius, q<sub>t</sub>
- scale radius of cloud in pc, l<sub>scale</sub>
- number density of hydrogen in all forms at the centre of the cloud (in cm<sup>-3</sup>),  $n_{\rm H,centre}$
- outer radii of each shell divided by *l*<sub>scale</sub>, *Q*<sub>shell</sub>. *Q*<sub>shell</sub> is calculated such that each shell has an equal mass of gas.
- mean thermal pressure in each shell, P<sub>therm</sub>
- $\tau_{\rm B}$  from the outer radius of each shell to the surface of the cloud. The outermost shell is always taken to be fully illuminated by the external radiation field.

- thermal pressure at centre of cloud, *P*<sub>centre</sub>
- $\tau_{\rm B}$  from the surface to the centre of the cloud

The ISM thermal/chemical model described in Chapter 3 is run iteratively within this cloud model, so that solutions for the line emissivities, gas temperature, molecular fraction and abundances of species are self-consistently obtained within each shell in the cloud. In particular, the CO (2–1) line emissivity from the output is compared to observations. This is discussed in Section 5.4. The following section describes the derivation of the total pressure in a galactic disc.

### 5.3.4 Total pressure in a galactic disc

In a galactic disc, the external pressure of pressure-supported clouds is defined by the thermal pressure of the diffuse warm ionised medium (WIM), mixed in with the warm neutral medium (WNM). It is given by

$$P_{\rm ext} = n(z) k_{\rm B} T, \tag{5.3}$$

where n(z) is the gas number density in the WIM in terms of the height above the galactic disc, *z*. Adopting a plane-parallel model for the ISM and assuming that gravity is dominated by the thin stellar disc, the density distribution of the WIM is

$$n(z) = n_0 e^{-z/z_{\text{gas}}},$$
 (5.4)

where  $n_0$  is the gas density at the mid-plane and

$$z_{\rm gas} = \frac{k_{\rm B}T}{2\pi G \,\Sigma_{\rm tot} \,m'},\tag{5.5}$$

where  $\Sigma_{tot}$  is the total surface density (stars and gas combined), *m* is the mass of a gas particle and *G* is Newton's gravitational constant. The full derivation of these equations can be found in Appendix **G**.

### 5.4 Results

### 5.4.1 Predicting X<sub>CO</sub> from model quantities

In our model, we divide the galactic plane of NGC 628 into annuli with galactocentric radii between *R* and  $\Delta R$  assuming axisymmetry. We denote the mass of a cloud as  $M_{cloud}$  and the number of clouds in an annulus as  $N_{cloud}$ . Here, we are assuming that all clouds in NGC 628 have the same mass. We then compare observed and predicted radial profiles of CO brightness with different hypothetical cloud masses. From the cloud model and the chemistry model, the CO line luminosity  $L_{CO}$  per cloud and  $f_{H_2}$  of a cloud are predicted from the input parameters  $u_{\nu}$ ,  $P_{ext}$ ,  $\zeta_p$ ,  $Z_{metal}$  and  $M_{cloud}$ , where  $f_{H_2}$  per cloud refers to the molecular fraction of the whole cloud (e.g. as shown in Figure 5.6 as a function of galactocentric radius and  $M_{cloud}$ ). The dust mass in an annulus of NGC 628,  $M_{dust}$ , was obtained from the output of the RT modelling of NGC 628 by Rushton et al. (2022) - it is strongly anchored by the dust surface brightness in the sub-millimetre. The mass of hydrogen in H I and H<sub>2</sub> combined in an annulus is related to  $M_{dust}$  by

$$M_{\rm H} = \frac{M_{\rm dust}}{F_{\rm gr} Z_{\rm metal}},\tag{5.6}$$

where  $Z_{\text{metal}}$  is the absolute metallicity as a function of galactocentric radius. Assuming that there is no H<sub>2</sub> outside clouds and referring to the "gas" panel in Figure 5.6, the mass of H<sub>2</sub> in an annulus  $M_{\text{H}_2}$  is  $M_{\text{H}_2} = M_{\text{H}} - M_{\text{H}_{\text{I}}}$ , where  $M_{\text{H}_{\text{I}}}$  is the observed H<sub>I</sub> mass from THINGS observations (Walter et al. (2008)).  $M_{\text{H}}$  is derived from  $\Sigma_{\text{gas}}$  in Figure 5.6 assuming the mass of H<sub>II</sub> in the galactic disc is negligible. The number of clouds in an annulus  $N_{\text{cloud}}$  can then be related to  $M_{\text{H}_2}$  by

$$N_{\rm cloud} = \frac{M_{\rm H_2}}{M_{\rm cloud} f_{\rm H_2}},\tag{5.7}$$

where  $f_{\text{H}_2}$  is a function of  $M_{\text{cloud}}$  predicted from the model. The predicted  $L_{\text{CO}}$  in an annulus from passive clouds is then equal to  $N_{\text{cloud}}$  multiplied by the emergent CO line luminosity per cloud predicted by the model,  $L_{\text{CO}}$ .  $X_{\text{CO}}$  is conventionally defined as  $X_{\text{CO}} \equiv N_{\text{H}_2}/W_{\text{CO}}$  and the denominator can be written as  $W_{\text{CO}} = T_{\text{B}}\Delta v$ , where  $T_{\text{B}}$  is the Rayleigh-Jeans brightness temperature and  $\Delta v$  the CO line width in km s<sup>-1</sup>. The line brightness is then equal to  $L_{\text{CO}}$  divided by the area of an annulus, and expressed in units of  $W_{\text{CO}}$ . This is then compared with observations (see Figure 5.8).

### 5.4.2 Model predictions



FIGURE 5.8: Model predictions of azimuthally averaged profiles of NGC 628. Panels for molecular fraction, gas temperature and free electron density are mass-weighted averages over the shells of each cloud model. Also plotted are the truncation radius and B-band optical depth as a function of the galactocentric radius. Curves for cloud masses of 3, 10, 30, 100, 300, 1000, 3000 and 10000 M<sub> $\odot$ </sub> (solar masses) are plotted. All calculations are for a fixed virial velocity parameter of  $v_{\rm vir} = 15 \,\rm km \, s^{-1}$ , which is the typical velocity dispersion observed for individual massive molecular clouds in NGC 628 by ALMA. The predicted range of cloud properties is similar to those observed in the interstellar medium.

Figure 5.8 shows the model predictions of molecular fraction, gas temperature, electron density, truncation radius, B-band optical depth and  $X_{CO}$  (2–1) as a function of galactocentric radius and cloud mass. The general trends are the increase of molecular fraction, decrease of gas temperature, and increase of  $\tau_B$  with increasing cloud mass. For the most massive cloud, 10000 M<sub> $\odot$ </sub>, virial support can only be provided for  $v_{vir} = 15 \text{ km s}^{-1}$ , for clouds situated at  $R \ge 5 \text{ kpc}$  (where R is the galactocentric radius). This is because at lower galactocentric radii, the external pressure is higher, forcing the clouds to be more compact than can be supported with  $v_{vir} = 15 \text{ km s}^{-1}$ .

As discussed in Section 1.2.3, the CO-to-H<sub>2</sub> conversion factor,  $X_{CO}$ , is often expressed in terms of the ratio of the H<sub>2</sub> column density  $N_{H_2}$  to the observed velocity-integrated intensity of CO (1–0) line emission. It has a typical value of  $\sim 2 \times 10^{20}$  cm<sup>-2</sup> (K km s<sup>-1</sup>)<sup>-1</sup> for the Milky Way disc, as determined from different methods (Bolatto, Wolfire, and Leroy (2013)), though the value has a variation of a factor of  $\sim$ 2. To distinguish this value from the  $X_{CO}$  factor resulting from the CO (2–1) line, I denote this value as  $X_{CO(1-0)}$ . The empirical ratio of CO (2–1) line intensity to the CO (1–0) line intensity is expressed as

$$R_{21} = \frac{W_{\rm CO(2-1)}}{W_{\rm CO(1-0)}},\tag{5.8}$$

where  $W_{CO(2-1)}$  is the observed velocity-integrated intensity of CO (2–1) line emission.

Figure 5.9 shows the model predictions of  $X_{CO(2-1)}$  as a function of galactocentric radius in NGC 628. There is a large variation in  $X_{CO(2-1)}$ , especially for lower cloud masses. Except for the highest cloud masses, the predicted  $X_{CO(2-1)}$  values shoot up beyond a critical galactocentric radius, depending on cloud mass. This is because the pressure decreases with increasing galactocentric radius, making the clouds more diffuse and emit less CO emission. This is especially the case for low cloud masses. Interior to this critical galactocentric radius, undulations in  $X_{CO(2-1)}$  are seen, which are due to systematic variations in the radiation field incident on the cloud and the external pressure.

In general, the  $X_{CO(2-1)}$  values are higher for lower mass clouds, because clouds of higher masses are more opaque (see Figure 5.8) and have a larger fraction of molecular mass which is under illumination by the ISRF.



FIGURE 5.9: Model predictions of  $X_{CO(2-1)}$  as a function of galactocentric radius in NGC 628. Curves for cloud masses of 3, 10, 30, 100, 300, 1000, 3000 and 10000 M<sub> $\odot$ </sub> are plotted. All clouds have a virial velocity of 15 km s<sup>-1</sup>.

### 5.4.3 Comparison with Sandstrom et al. (2013)

Assuming the dust-to-gas ratio is approximately constant on kiloparsec scales, Sandstrom et al. (2013) provided solutions of  $\alpha_{CO(1-0)}$  in nearby galaxies including NGC 628.  $\alpha_{CO(1-0)}$  relates the H<sub>2</sub> surface density to the CO (1-0) line intensity via  $\Sigma_{H_2} = \alpha_{CO(1-0)} W_{CO(1-0)}$ . Including a factor of 1.36 for helium,

$$X_{\rm CO(1-0)} = 2 \times 10^{-20} \,\rm cm^{-2} \,(K \,\rm km \, s^{-1})^{-1} \tag{5.9}$$

corresponds to

$$\alpha_{\rm CO(1-0)} = 4.35 \,\rm M_\odot \, pc^{-2} \, (\rm K \, km \, s^{-1})^{-1}. \tag{5.10}$$

Using this conversion and a constant value of  $R_{21} = 0.7$ , Sandstrom et al. (2013) found

$$1.5 \times 10^{-20} \text{ cm}^{-2} \text{ (K km s}^{-1})^{-1} \leq X_{\text{CO}(2-1)} \leq 3.3 \times 10^{-20} \text{ cm}^{-2} \text{ (K km s}^{-1})^{-1} \tag{5.11}$$

for  $0 \le R \le 5.6$  kpc in NGC 628. For a given cloud mass, our predictions of  $X_{CO(2-1)}$  have a high dispersion and are lower than this range before the shoot-up. Potential reasons for this will be given in Section 5.4.6.

### 5.4.4 Comparison with Shetty et al. (2011b)

Using magnetohydrodynamic simulations and simple RT calculations, Shetty et al. (2011b) found cloud-averaged values of  $X_{CO(1-0)} = 2-4 \times 10^{20} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1}$ 

for temperatures  $T \sim 10-20$  K, velocity dispersions  $\sigma_v \sim 1-6$  km s<sup>-1</sup> and  $N_{\text{H}_2} \sim 2-20 \times 10^{21}$  cm<sup>-2</sup> for solar-metallicity models. Assuming  $R_{21} = 0.7$ , this is equivalent to  $2.9 \times 10^{20}$  cm<sup>-2</sup> (K km s<sup>-1</sup>)<sup>-1</sup>  $\leq X_{\text{CO}(2-1)} \leq 5.7 \times 10^{20}$  cm<sup>-2</sup> (K km s<sup>-1</sup>)<sup>-1</sup>. Our predicted  $X_{\text{CO}(2-1)}$  values are lower than this in general. It could be due to the fact that the range of velocity dispersion used in Shetty et al. (2011b) is much lower than our value of 15 km s<sup>-1</sup>, as Shetty et al. (2011b) found  $X_{\text{CO}(1-0)} \propto \sigma_v^{-1/2}$  for  $\sigma_v = 2-20$  km s<sup>-1</sup>.

### 5.4.5 Model prediction of CO (2–1) line emission



FIGURE 5.10: Comparison of the emergent CO (2–1) line emission predicted by the model and the observed CO (2–1) emission. Curves for cloud masses of 3, 10, 30, 100, 300, 1000, 3000 and 10000  $M_{\odot}$  are plotted. All clouds have a virial velocity of 15 km s<sup>-1</sup>.

Figure 5.10 shows the comparison of the predicted CO (2–1) line brightness from the model for different assumed cloud masses with the observed CO (2–1) line brightness by HERACLES (dashed line, equivalent to the dashed line in Figure 5.5). The variation of observed CO line brightness with galactocentric radius is well reproduced for the  $10^4 M_{\odot}$  cloud model, though it overpredicts the observed relation by a factor of 2. For lower mass clouds the overprediction is higher. For a given cloud mass, there is a sudden drop-off in the predicted CO line brightness beyond a certain galactocentric radius since the low ambient pressure in the outer galaxy makes the gas more diffuse, thus inhibiting the formation of CO.

### 5.4.6 Reasons for overprediction of CO line emission

The following discusses some potential reasons for the overprediction of CO line emission in NGC 628:

- 1. **Dust emissivity is overestimated in the Weingartner and Draine (2001a) model** If the dust emissivity is overestimated, the dust mass is overestimated. Through the dust-to-gas ratio, the gas mass is then also overestimated by the model, leading to an overprediction of the CO line emission. The physical reason is that the Weingartner and Draine (2001a) dust model has been calibrated on translucent clouds. It may not be applicable to dust in opaque clouds, where ice mantles can form, increasing the dust emissivity.
- 2. Real interstellar clouds are not perfectly spherical in shape, but has hierarchical structure such as clumps and cores (see Figure 5.11)

As mentioned, real clouds are clumpy, unlike the idealised homogeneous model used here. Illumination of gas will be maximised in a homogeneous model, and the cloud is more transparent. This will tend to lead to an overprediction of  $L_{CO}$ , also supported by numerical simulations (e.g. Shetty et al. (2011a)). If the CO emission zones in the cloud in Figure 5.11 are located in the clumps or cores, the CO emission cannot escape more easily than from a spherical cloud, since the CO-producing regions in the inhomogeneous cloud are more opaque.



FIGURE 5.11: Cartoon showing the hierarchical structure of a molecular cloud. The image is not drawn to scale. Figure taken from Pokhrel et al. (2018) under a Creative Commons Attribution 3.0 licence

# 3. The calculation is incomplete and it needs to be iterated with the large scale RT solution for NGC 628

The issue here is that if a large fraction of the gas in galaxies is in opaque passive clouds, the Popescu et al. (2011) model, as applied to NGC 628 by Rushton et al. (2022) will not take this into account, because it assumes all opaque clouds are associated with star-forming regions. All dust not associated with star-forming regions is taken to be transparent to UV on parsec scales. This will lead to a lower derived star formation rate and lower UV incident on the clouds then predicted by Rushton et al. (2022). We expect the UV radiation field will be lowered when running large scale RT with the cloud pseudograins presented here, which are very optically thick. This will reduce the predicted CO line emission. Reabsorption of dust-radiated light in the clouds will be important.

### 4. The effects of CRs on gas chemistry require further investigation

Increased CR flux will make the CO lines brighter and the cloud more transparent due to the increase in gas temperature and decrease in gas density. At the same time, as discussed in Section 3.14.3, increased cosmic ray ionisation will decrease the CO abundance. These competing effects require further investigation. Moreover, especially for massive clouds, gas in the interior regions of clouds is mainly heated by CRs. If CR flux is higher in the centres of galaxies, this will affect the  $X_{CO}$  ratio for these clouds.

Among the 4 reasons, the first reason is the most probable. This suggests a reexamination of the dust emissivity in the Weingartner and Draine (2001a) dust model in the future. The fourth reason may be important too, as high ionisation rates ( $2-7 \times 10^{-15} \text{ s}^{-1}$ ) have been predicted for the central molecular zone (CMZ) in the Milky Way based on observations of H<sup>+</sup><sub>3</sub> (Oka et al. (2005)). Although it was recently suggested that this high value of ionisation rate cannot be fully explained by cosmic rays (Ravikularaman et al. (2024)), it is very possible that CR flux has a major impact on gas chemistry in the CMZ. Similar effects may also occur in the centres of external galaxies and further investigation is required.

# Chapter 6

# Summary and outlook

### 6.1 Summary

The main new results described in this thesis are:

- In Chapter 2, I have extended existing computations of the PE heating by starlight to include PE heating by NUV and optical light, rather than just FUV light as previously. In Chapter 3, I showed that indeed optical PE heating becomes a major source of gas heating in highly obscured regions of the ISM such as those encountered in interstellar clouds.
- 2. In Chapter 3, I developed a new chemistry model, building on previous formulations but only considering the principle heating and cooling channels. This allowed analytic approximations which allow for high computational speed without compromising accuracy, making the code suitable for integrating with complex RT calculations of propagation of photons in the ISM and in clouds. Without loss of speed, I extended this model to take into account pressure support by CRs and magnetic field in addition to thermal pressure support in Chapter 4.
- 3. In Chapter 3, I explored the circumstances by which CRs would directly affect CO line emissivity in the ISM. I showed that, by virtue of the extra electrons that lower grain charge, ionisation of the ISM by CRs lowers the photoemission threshold energy and thereby boosts the PE heating rate. This is a catalytic effect of CRs, since it arises independently of the boost of CO line luminosity due to direct heating of gas by CR. I also showed in Chapter 3 that the latter effect of CR heating of gas is also important in affecting the CO line emission, typically for CR ionisation rates of  $10^{-15}$  s<sup>-1</sup> or more, which may for example apply in the inner regions of the Milky Way.
- 4. In Chapter 5, I integrated my simple chemical model with spherically symmetrical models of interstellar clouds in hydrostatic equilibrium, applying a self-consistent treatment of radiative transfer of stellar light and light in spectral lines, to predict the luminosity of emergent lines as a function of cloud mass (which only has one free parameter  $M_{cloud}$ ). The models were used to

predict the  $X_{CO}$  factor relating the mass of H<sub>2</sub> to flux in the CO (2–1) line for clouds illuminated by the diffuse ISRF in the nearby spiral galaxy NGC 628, resulting in  $X_{CO}$  factors within a factor of 2 of those obtained by sophisticated hydrodynamical models. Applying the model to observations of the CO (2–1) line emission of clouds in NGC 628, and taking into consideration only the line heating by ISRF, I derived surface densities of H<sub>2</sub> which are lower by a factor of ~2 compared with estimates of H<sub>2</sub> mass based on the emission of dust in the galaxy. This discrepancy would be even larger if lower  $X_{CO}$  factors were applied, or if CR heating would be taken into account, but could be accounted for if the emissivity of dust is overestimated by the dust models used in the RT analysis.

## 6.2 Outlook

### 6.2.1 The need for a representative cloud model

A main goal of this work was to create a primitive model framework for predicting CO line emission from molecular gas (as may be the case) heated by the diffuse ISRF, partially supplemented by the heating of CRs. As I showed in Chapter 5, on the basis of an idealised spherically symmetric model of clouds, one can quantify the relation of ISRF to CO line emission, but this effect is dominated by the mass of the cloud, since it is the latter that controls the penetration of light into the cloud and the chemical balance between  $H_2$  and  $H_1$ .

Therefore, it will be critical to create models of clouds representative of actual clouds to achieve a robust predictive power to measure  $H_2$  masses of clouds in galaxies. It can in principle be achieved in two ways. Firstly, by performing magnetohydrodynamical simulations of the formation of clouds. However, even today, the resolutions of such simulations cannot reach the critical scales where, for example turbulent energy is converted into heat. Moreover, many input parameters are needed, producing a wide range of outcomes.

A second complementary approach, the seeds of which I have laid in this thesis, will be to use simple semi-analytic descriptions of clouds, and capture their parameters such that a wide variety of predicted emission of dust and line emission fits observations of clouds. As observational templates, local clouds in the vicinity of the Sun, for example as measured by Cahlon et al. (2024) would be a possible starting point for the development of such models, because these have a high linear resolution with an analytic description of structural components, and the optical depth effects controlling the escape of line photons can thereby be empirically constrained. On the modelling side, because much substructure is observed to be filamentary, cylindrical geometry, rather than the spherical geometry as adopted in Chapter 5, would be a possible starting point. The addition of cylindrical substructures according to data would be required, such that the resolved images of CO line emission can be reproduced.

A further advantage of using a local cloud as the basis of an empirically constrained model, is that, because the local CR flux is known, we can use the gamma-ray ( $\gamma$ -ray) emission to directly constrain the H<sub>2</sub> mass, especially if measured at high enough energy that we can ignore CR propagation effects (e.g.  $\gtrsim 100$  GeV). This will, for example, enable us to directly constrain dust emissivities, giving us a handle to investigate the relation of grain emissivity to conditions of illumination inside the cloud.

The latter approach will be particularly important when data on clouds from the new SPHEREx IR spectroscopy mission (to be launched in 2025<sup>1</sup>) becomes available, as this will enable detailed measurements of the structure of local clouds at high optical depth to be made, combining measurements of mid-infrared (MIR) extinction and MIR-FIR<sup>2</sup>-submillimetre emission. In reality, one of the biggest unknowns is the physical and chemical properties of grains and large molecules, which will influence greatly the heating and cooling of gas. Especially due to the inhomogeneous nature of molecular clouds, it is very challenging to build *ab initio* models which are physically and chemically self-coupled, so an empirical approach is attractive.

### 6.2.2 Tracing low and high energy cosmic rays in clouds

One of the main results in this thesis was the prediction that the  $X_{CO}$  factor is likely to depend on the heating of the ISM by low energy CRs, especially in the inner regions of the Milky Way. This potentially may systematically affect the inference of flux of high energy CRs in the ISM from measurements of very high energy (TeV range)  $\gamma$ -rays from pions produced in collisions of CRs with molecular gas in the ISM. It will therefore be important to provide direct observational tracers of CR ionisation of those clouds used to elucidate the high energy CR flux from GeV–TeV measurements of  $\gamma$ -rays. In the past, tracers such as  $H_3^+$  (see e.g. the review by Gabici (2022)) have been proposed. However, this line is heavily dependent on the molecular fraction, and therefore the mass of the cloud. A more universal indicator would potentially be the He I recombination lines, which are also available as an optically thin probe at radio wavelengths. At the same time, effects of X-ray ionisation on ionisation rate would need to be considered.

In terms of the cloud models, it will be necessary to explicitly calculate the propagation of CRs penetrating the cloud in both spatial and momentum space. This is analytically reasonable for isotropic distributions of external CRs propagating in highly

 $<sup>^1 {\</sup>tt see https://spherex.caltech.edu}$  for the current status of the mission

<sup>&</sup>lt;sup>2</sup>FIR stands for far infrared

ordered magnetic fields, but would need numerical simulations for anisotropic magnetic fields. One would also need to incorporate the extreme UV (EUV) external radiation field into models, to predict the component of recombination line emission energy from external ionising radiation fields incident onto the clouds. In addition, the FUV fluorescence triggered inside the clouds by CR ionisation needs to be taken into account (see e.g. Prasad and Tarafdar (1983)). This would offer a different intrinsic ratio of H and He recombination lines, enabling the CR-powered and the EUV powered components of the ionisation to be distinguished.

### 6.2.3 Final remarks

As a final conclusion, my work indicates that global modelling of  $\gamma$ -ray emission from CRs in galaxies very probably requires a multi-wavelength approach (incorporating measurements and models for radiation fields, clouds, and line emission), to robustly measure the distribution of gas targets for the production of  $\gamma$ -rays via the pion decay mechanism. Deep measurements of radio recombination lines of the Milky Way by the *Square Kilometre Array* (Dewdney et al. (2009)) could provide such data. As measurements of the spatial and energy distribution of  $\gamma$ -rays are available for the galactic plane of the Milky Way (e.g. The High Energy Spectroscopic System (H.E.S.S.) (H.E.S.S. Collaboration (2018)), this could be the first step to solve the inverse problem of inverting  $\gamma$ -ray observations to constrain the spatial and energy distribution of CRs in galaxies, offering another route instead of *ab initio* calculations of CR propagation.

# Appendix A

# Weingartner & Draine (2001) PE heating model

# A.1 Introduction

Building on the previous models, the Weingartner and Draine (2001b) model (WD01b) is the most sophisticated model for PE heating to date. This section summarises the concepts and quantities used in this model.

# A.2 Photoemission threshold energy

The photoemission threshold energy  $hv_{pet}$  is the minimum energy for which an incident photon can initiate the photoelectric effect on a certain dust grain. It depends on the work function W of the grain (which depends on the grain composition; for carbonaceous grains, W = 4.4 eV, whereas W = 8.0 eV for silicate grains), the grain charge Z, the grain size and the photon energy (hv). Here, to simplify the calculations, it is assumed that all dust grains are spherical in shape with radius a, although small PAHs are planar molecules in reality.

# A.3 Ionisation potential and electron affinity

The ionisation potential (IP) is the difference in energy between infinity and the highest occupied state. When the charge of the grain *Z* is negative (*Z* < 0), the "extra" electrons, which occupy the "lowest unoccupied molecular orbital" (LUMO) of the neutral, are separated from the top of the valence band by the band gap, with extra energy  $E_{bg}$  (assuming the valence band is full in the neutral). The electron affinity EA(*Z*) is the difference in energy between infinity and the LUMO for the grain of charge (*Z* - 1)*e* created by adding the electron. Thus, IP(*Z* < 0) = EA(*Z* + 1). We can also define the "valence band ionisation potential" IP<sub>V</sub>(*Z*), equal to the difference in energy between infinity and the top of the valence band. Of course, IP<sub>V</sub>(*Z*) = IP(*Z*) when *Z* ≥ 0. Empirically, IP<sub>V</sub>(*Z*) can be fitted by

$$IP_{V}(Z) = W + \left(Z + \frac{1}{2}\right)\frac{e^{2}}{a} + (Z + 2)\frac{e^{2}}{a}\frac{0.3 \text{ Å}}{a}$$
(A.1)

with the graphite work function W = 4.4 eV and *a* is the radius of the grain<sup>1</sup>. This value is taken to be the work function for carbonaceous grains. For silicate grains, W = 8.0 eV. Equation A.1 is used to calculate IP<sub>V</sub> for both carbonaceous and silicate grains.

For carbonaceous grains, the electron affinity can be approximated by

$$EA(Z) = W + \left(Z - \frac{1}{2}\right)\frac{e^2}{a} - \frac{e^2}{a}\frac{4 \text{ Å}}{a + 7 \text{ Å}},$$
 (A.2)

while for silicates,

$$EA(Z) = W - E_{bg} + \left(Z - \frac{1}{2}\frac{e^2}{a}\right)$$
(A.3)

with  $W - E_{bg} = 3 \text{ eV}$ .

# A.4 Photoemission threshold

It is assumed that, when Z < 0, the highest occupied energy level is very close to the top of the valence band, since the number of electrons that have been removed from the grain is small compared with the total number of electrons in the grain. Thus, for  $Z \ge 0$ , the threshold photon energy for photoelectric emission is given by  $hv_{pet}(Z) = IP_V(Z) = IP(Z)$ . When Z < -1,  $hv_{pet}(Z) > IP(Z)$  because the electron has to overcome the repulsive Coulomb barrier. Suppose the tunnelling probability becomes significant when the electron energy exceeds the potential at infinity by  $E_{min}$ . Then  $hv_{pet}(Z) = IP_V(Z) + E_{min}$ . Thus, we take

$$h\nu_{\rm pet}(Z,a) = \begin{cases} {\rm IP}_V(Z,a), & Z \ge -1, \\ {\rm IP}_V(Z,a) + E_{\rm min}(Z,a), & Z < -1. \end{cases}$$
(A.4)

The following expression is adopted for  $E_{\min}$ , which reproduces the results of the Wentzel-Kramers-Brillouin (WKB) approximation fairly well:

$$E_{\min}(Z < 0, a) = -(Z+1)\frac{e^2}{a} \left[1 + \left(\frac{27 \text{ Å}}{a}\right)^{0.75}\right]^{-1}$$
(A.5)

## A.5 Photoelectric yield

The photoelectric yield Y is the probability that an electron will be ejected following the absorption of a photon. Fundamentally, Y is dependent on four factors: (1) the grain composition (carbonaceous or silicate), since the material of the grain determines the optical properties of the grain; (2) the energy of the photon (hv), which

<sup>&</sup>lt;sup>1</sup>One can express *e* in cgs units as  $e = 4.8 \times 10^{-10}$  esu and *a* in cm.  $e^2/a$  can then be calculated in ergs, which can be converted into eV for ease of calculation.

largely determines whether the photon has more energy than the photoemission energy; (3) the grain charge Z (Y increases with lower Z); (4) radius of the grain a (in general, Y decreases with higher a).

WD01b first defined the yield  $y'_0$  of electrons that traverse the surface layer, emerge from the grain surface, and have enough energy to overcome the image potentials (called "attempting" electrons). For Z < 0, every attempting electron will escape, but when  $Z \ge 0$ , some of these electrons have insufficient energy to escape to infinity and instead fall back to the grain.  $y'_0$  is assumed to have the form of:

$$y_0' = y_0(\Theta)y_1(h\nu, a) \tag{A.6}$$

where the parameter  $\Theta$  is given by

$$\Theta = \begin{cases} h\nu - h\nu_{\text{pet}} + (Z+1)e^2/a, & Z \ge 0, \\ h\nu - h\nu_{\text{pet}}, & Z < -1. \end{cases}$$
(A.7)

and the factor  $y_1(h\nu, a)$  accounts for the size-dependent geometrical yield enhancement discussed above;  $y_1$  depends on  $h\nu$  because the photon attenuation length  $l_{\alpha}$  does.

It is assumed that the attempting electrons have a parabolic energy distribution:

$$f_{\rm E}^0(E) = \frac{6(E - E_{\rm low})(E_{\rm high} - E)}{(E_{\rm high} - E_{\rm low})^3},$$
(A.8)

where  $f_E^0(E)dE$  gives the fraction of attempting electrons with energy (with respect to infinity) between *E* and *E* + d*E*. When *Z* < 0,  $E_{\text{low}} = E_{\text{min}}$  and  $E_{\text{high}} = E_{\text{min}} + h\nu - h\nu_{\text{pet}}$ ; when *Z* ≤ 0,  $E_{\text{low}} = -(Z+1)e^2/a$  and  $E_{\text{high}} = h\nu - h\nu_{\text{pet}}$ .

Let  $y_2 \leq 1$  be the fraction of attempting electrons that escape to infinity:

$$y_{2}(h\nu, Z, a) = \int_{\max(0, E_{\text{low}})}^{E_{\text{high}}} f_{\text{E}}^{0}(E) dE$$
(A.9)

$$=\begin{cases} \frac{E_{\text{high}}(E_{\text{high}}-3E_{\text{low}})}{(E_{\text{high}}-E_{\text{low}})^3}, & Z \ge 0, \\ 1, & Z < 0. \end{cases}$$
(A.10)

The resulting expression for the photoelectric yield is

$$Y(h\nu, Z, a) = y_2(h\nu, Z, a) \min[y_0(\Theta)y_1(a, h\nu), 1].$$
(A.11)

Draine's estimation of the expression for  $y_1$ , which approximately reproduces results based on Mie theory, is:

$$y_1 = \left(\frac{\beta}{\alpha}\right)^2 \frac{\alpha^2 - 2\alpha + 2 - 2e^{-\alpha}}{\beta^2 - 2\beta + 2 - 2e^{-\beta}}$$
(A.12)

where  $\beta = a/l_a$  and  $\alpha = a/l_a + a/l_e$ .  $l_e$  is the electron escape length and is taken to be  $l_e = 10$  Å, independent of energy. The photon attenuation length  $l_a$  is given by

$$l_{\rm a} = \frac{\lambda}{4\pi \,{\rm Im}(m(\lambda))} \tag{A.13}$$

where  $\lambda$  is the wavelength in vacua and  $m(\lambda)$  is the complex refractive index. Since graphite is a highly anisotropic material and has a dielectric function in tensor form, for carbonaceous grains, the  $l_a$  is taken as

$$l_{\rm a}^{-1} = \frac{4\pi}{\lambda} \left[ \frac{2}{3} \, {\rm Im}(m_{\perp}) + \frac{1}{3} \, {\rm Im}(m_{\parallel}) \right] \tag{A.14}$$

where  $m_{\perp}$  and  $m_{\parallel}$  are for the electric field perpendicular and parallel to the *c*-axis, respectively.

 $y_0(\Theta)$  for carbonaceous grains is

$$y_0(\Theta) = \frac{9 \times 10^{-3} (\Theta/W)^5}{1 + 3.7 \times 10^{-2} (\Theta/W)^5}$$
(A.15)

with W = 4.4 eV. For silicate grains, it is

$$y_0(\Theta) = \frac{0.5(\Theta/W)}{1 + 5(\Theta/W)} \tag{A.16}$$

with W = 8 eV.

# A.6 Photoelectric ejection of attached electrons (photodetachment)

When Z < 0, the -Z attached electrons occupy energy levels above the valence band, if the latter is full in the neutral. The photodetachment threshold energy  $hv_{pdt}$  is taken to be

$$h\nu_{\rm pdt}(Z < 0) = {\rm EA}(Z + 1, a) + E_{\rm min}(Z, a),$$
 (A.17)

with electron affinities EA given by Equations A.2 and A.3, and  $E_{min}$  by Equation A.5. WD01b assumed that  $E = hv - hv_{pdt}$  for photodetached electrons since attached electrons lie in a narrow range of energies.

WD01b assumed that an oscillator strength  $f_{pdt}$  is associated with photodetachment

transitions to the continuum. The photodetachment cross section  $\sigma_{pdt}(h\nu)$  can be roughly approximated by

$$\sigma_{\rm pdt}(h\nu, Z, a) = -Z \, \frac{2\pi e^2 h f_{\rm pdt}}{3m_{\rm e} c\Delta E} \frac{x}{(1+x^2/3)^2},\tag{A.18}$$

where  $x \equiv (h\nu - h\nu_{pdt})/\Delta E$ , and the peak in  $\sigma_{pdt}$  occurs at  $h\nu = h\nu_{pdt} + \delta E$ . They take  $\Delta E = 3 \text{ eV}$  and oscillator strength  $f_{pdt} = 0.5$ . Thus,

$$\sigma_{\rm pdt}(h\nu, Z, a) = 1.2 \times 10^{-17} \,{\rm cm}^2 \,|Z| \,\frac{x}{(1+x^2/3)^2} \quad {\rm for} \, Z < 0.$$
 (A.19)

# A.7 Grain charge distributions

Since the photoemission depends on the grain charge, it is necessary to know the distribution of charge states for the grains. In statistical equilibrium,

$$f_Z(Z)J_{pe}(Z) = f_Z(Z+1)J_e(Z+1)$$
 (A.20)

where  $f_Z(Z)$  is the probability for the grain charge to be Ze,  $J_{pe}$  is the photoemission rate and  $J_e$  is the electron accretion rate. WD01b's model also includes a  $J_{ion}$  term on the left hand side, denoting the positive ion accretion rate (e.g. accretion of protons onto the grains), but it is neglected here because of the large proton mass relative to the electron. Also, it is assumed that the number density of electrons is far greater than that of protons ( $n_e \gg n_p$ ), meaning that the proton accretion rate is negligible compared to the electron accretion rate.

The most positive and the most negative charges that a grain could possible acquire  $(Z_{\text{max}}e \text{ and } Z_{\text{min}}e, \text{ respectively})$  should be considered. The most positive charge is one proton charge more than the highest charge for which an electron can be ejected, i.e., for which  $hv_{\text{pet}} = \text{IP} < hv_{\text{max}}$ , the maximum photon energy in the radiation field (=13.6 eV, in an H<sub>I</sub> region). Thus,

$$Z_{\max} = \inf\left[\left(\frac{h\nu_{\max} - W}{14.4 \text{ eV}}\frac{a}{\text{\AA}} + \frac{1}{2} - \frac{0.3 \text{\AA}}{a}\right)\left(1 + \frac{0.3 \text{\AA}}{a}\right)^{-1}\right]$$
(A.21)

where int[x] denotes the greatest integer less than x. The minimum allowed charge  $Z_{min}e$  is the most negative charge for which autoionisation does not occur. The autoionisation threshold potential  $U_{ait}$  is taken to be that at which the electron current is  $\approx 10^{-6} \text{ s}^{-1}$ . WD01b evaluated the tunnelling probability using the WKB approximation and assume an attempt frequency of  $\approx 2 \times 10^8 \text{ s}^{-1}(\text{cm})/a$ . They found that

$$\frac{-U_{\text{ait}}}{V} \approx \begin{cases} 3.9 + 0.12(a/\text{\AA}) + 2(\text{\AA}/a) & \text{for carbonaceous,} \\ 2.5 + 0.07(a/\text{\AA}) + 8(\text{\AA}/a) & \text{for silicate.} \end{cases}$$
(A.22)

this agrees very well with Draine & Salpeter's (1979) estimate of the potential at which field emission becomes important. The most negative allowed charge is than given by

$$Z_{\min} = \operatorname{int}\left(\frac{U_{\operatorname{ait}}}{14.4\,\operatorname{V}}\frac{a}{\operatorname{\AA}}\right) + 1 \tag{A.23}$$

By iteratively applying Equation A.20 and normalising,  $f_Z$  can be found for all Z.

# A.8 Photoemission rate

The photoemission rate is given by

$$J_{\rm pe}(a,Z) = \pi a^2 \int_{\nu_{\rm pet}}^{\nu_{\rm max}} Y(h\nu,a,Z) Q_{\rm abs}(\nu) \frac{c u_{\nu}}{h\nu} \,\mathrm{d}\nu \tag{A.24}$$

$$+ \int_{\nu_{\text{pdt}}}^{\nu_{\text{max}}} \sigma_{\text{pdt}}(\nu) \frac{cu_{\nu}}{h\nu} \, \mathrm{d}\nu \tag{A.25}$$

where  $Q_{abs}$  is the absorption efficiency,  $u_{\nu}$  is the radiation energy density per frequency interval, and *c* is the speed of light. The second term in the above equation is only present when Z < 0.

## A.9 Electron accretion rate

The accretion rate is given by

$$J_{\rm e}(Z) = n_{\rm e}s_{\rm e}(Z) \left(\frac{8kT}{\pi m_{\rm e}}\right)^{1/2} \pi a^2 \tilde{J}(\tau_{\rm e},\xi_{\rm e}) \tag{A.26}$$

where  $n_e$  is the electron density,  $s_e$  is the sticking coefficient of electron, which is the probability that an electron will transfer its charge if it reaches the surface of a grain of charge Ze,  $m_e$  is the electron mass, T is the gas temperature, and  $\tilde{J}$  is a function of  $\tau_e \equiv akT/e^2$  and  $\xi_e \equiv -Z$  (k is the Boltzmann constant). Expressions for  $\tilde{J}$  can be found in Draine and Sutin (1987).

## A.10 Sticking coefficients

A low-energy electron impinging on a macroscopic solid surface has some probability  $p_{\rm es}$  of elastic scattering. WD01b assumed that  $p_{\rm es} \approx 0.5$ , so that the maximum possible value of the sticking coefficient  $s_{\rm e}$  would be  $(1 - p_{\rm es} \approx 0.5)$ .

We first consider electron attachment to neutral grains. If the electron affinity EA > 0, then the approaching electron accelerates because of its polarisation of the grain,

arriving at the surface with a kinetic energy of order EA. Even if it enters the grain material (with probability  $(1 - p_{es})$ ), the electron may fail to undergo an inelastic scattering event, in which case it passes through the grain and returns to infinity. The probability of undergoing inelastic scattering is approximately  $(1 - e^{-a/l_e})$ , where  $l_e \approx 10$  Å, the "electron escape length", is roughly the mean free path against inelastic scattering within the grain material. The electron attachment sticking coefficient can then be written as the product of three factors:

$$s_{\rm e}(Z=0) \approx (1-p_{\rm es})(1-{\rm e}^{-a/l_{\rm e}})p_{\rm rad}$$
 (A.27)

where  $p_{rad}$  is the probability of "radiative stabilisation" of the negatively charged grain, i.e., the probability of radiating away  $\sim kT$  of energy before the electron is ejected. We expect  $p_{rad} \rightarrow 1$  for macroscopic grains but  $p_{rad} < 1$  for grains with a small number of internal degrees of freedom. Thus, the sticking coefficient can be expressed as

$$s_{\rm e}(Z=0) = 0.5(1-{\rm e}^{-a/l_{\rm e}})rac{1}{1+{\rm e}^{(20-N_{\rm C})}}$$
 (A.28)

where  $N_{\rm C}$  is the number of atoms other than H in the molecule and  $l_{\rm e} = 10^{-7}$  cm.

For the case of electrons attaching to negatively charged grains, as a grain acquires more electrons, the electron affinity decreases. We take the sticking coefficient to be zero when  $Z = Z_{min}$  since the more negatively charged state, even if it formed, would autoionise. Thus,

$$s_{\rm e}(Z < 0) = \begin{cases} s_{\rm e}(Z = 0), & Z > Z_{\rm min} \\ 0, & Z \le Z_{\rm min} \end{cases}$$
(A.29)

Electrons arriving at positively charged grains are expected to recombine provided that

(1) they do not reflect elastically from the surface, and

(2) they are able to scatter inelastically before traversing the grain. For hydrocarbons, this most likely results in only the loss of an H atom, with the carbon skeleton remaining intact. The sticking coefficient is therefore expected to be

$$s_{\rm e}(Z > 0) \approx (1 - p_{\rm es})(1 - e^{-a/l_{\rm e}}) \approx 0.5(1 - e^{-a/l_{\rm e}})$$
 (A.30)

# A.11 Calculation of the total PE heating rate

For the calculation of the total PE heating rate, please see Section 2.3.10.
## Appendix **B**

## **Reactions in chemical network**

#### **B.1** List of chemical reactions in chemical network

The table on the next page shows the ionisation balance reactions from Glassgold and Langer (1974), which are used in full in my ISM model. Unless otherwise specified, all rate coefficients are taken from UMIST2012 astrochemistry database. *T* is in unit of K. For photoionisation and photodissocation reactions whose rate coefficients are taken from the UMIST database (reactions with rate coefficients  $k_7$ ,  $k_{18}$  and  $k_{19}$ ), since the UMIST database uses the Draine (1978) ISRF to calculate the photorates, the coefficients here have been multiplied by the factor (1.14/1.69). This is because the strength of the FUV field in the Draine (1978) ISRF is equal to 1.69 *G*<sub>0</sub> and the strength of the FUV field in the Mathis ISRF is equal to 1.14 *G*<sub>0</sub> (Draine (2011)).

| Reaction  | Rate coefficient   |
|---|--|
| Grain formation of H <sub>2</sub> :   |  |
| $H + H \longrightarrow H_2$   | $k_1 = R_{\rm H_2} / n_{\rm H}$ ; see Section 3.7.1  |
| Photodissociation of H <sub>2</sub> :   |  |
| $H_2 + \gamma \longrightarrow 2H$   | $k_2 = 4.92 \times 10^{-11} G_{\rm FUV}  {\rm s}^{-1}  ({\rm Draine}  (2011))^1$                                     |
| Cosmic-ray ionisation:  |  |
| $CRp + H \longrightarrow H^+ + e^- + CRp$   | $k_3=1.5\zeta_{ m p}$ (Glassgold and Langer (1974))  |
| $CRp + H_2 \longrightarrow H_2^+ + e^- + CRp$   | $k_4=2.3\zeta_{ m p}$ (Glassgold and Langer (1974))  |
| $\begin{array}{l} CRp + H_2 \longrightarrow H + H + CRp \\ CRe + H_2 \longrightarrow H + H + CRe \end{array}$ | $k_5 = 1.15  \zeta_{ m p}$ (Glassgold and Langer (1974))   |
| $CRp + He \longrightarrow He^+ + e^- + CRp$   | $k_6 = 1.5 \zeta_{ m p}$ (Glassgold and Langer (1974))   |
| Photoionisation:  |  |
| $C+\gamma \longrightarrow C^+ + e^-$  | $k_7 = 2.09 \times 10^{-10} \ G_{\rm FUV} \ { m s}^{-1}$   |
| Radiative recombination:  |  |
| $e^- + H^+ \longrightarrow H + \gamma$  | $k_8 = 3.5 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.75} \mathrm{cm}^3 \mathrm{s}^{-1}$                         |
| $e^- + H e^+ \longrightarrow H e + \gamma$  | $k_9 = 5.36 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.5} \text{ cm}^3 \text{ s}^{-1}$                           |
| $e^- + C^+ \longrightarrow C + \gamma$  | $k_{10} = 2.36 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.29} \mathrm{e}^{17.6/T} \mathrm{cm}^3 \mathrm{s}^{-1}$ |
| Dissociative recombination:   |  |
| $e^- + H_2^+ \longrightarrow 2H$  | $k_{11} = 1.6 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.43} \text{ cm}^3 \text{ s}^{-1}$                         |
| $e^- + H_3^+ \longrightarrow H_2 + H$   | $k_{12} = 2.34 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52} \text{ cm}^3 \text{ s}^{-1}$                        |
| $e^- + H_3^+ \longrightarrow 3H$  | $k_{13} = 4.36 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52} \text{ cm}^3 \text{ s}^{-1}$                        |
| Charge exchange:  |  |
| $H_2^+ + H \longrightarrow H_2 + H^+$   | $k_{14} = 6.4 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$   |
| Ion-molecule reaction:  |  |
| $H_2^+ + H_2 \longrightarrow H_3^+ + H$   | $k_{15} = 2.08 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$   |

 $<sup>^{-1}</sup>k_2 \approx 4 \times 10^{-11} \ \chi \ {
m s}^{-1}$ , where  $\chi = 1.23$  for the Mathis et al. (1983) ISRF

# B.2 Reactions relevant to the formation and destruction of CO

The following shows the reactions relevant to the formation and destruction of CO, which are not included in the GL74 chemical network.

Following Nelson and Langer (1997), it is assumed that CO is produced in the following way:

 $C^+$  reacts with  $H_2$  to form  $CH_2^+$ , which is then rapidly converted to CH by its reaction with  $H_2$  and dissociative recombination with  $e^-$ . The newly formed CH either reacts with O to form CO or is photodissociated by FUV photons. Therefore, the concentration of CH is negligible and it is not tracked in this model.

| $C^+ + H_2 \longrightarrow CH_2^+$  | $k_{16} = 2.6 \times 10^{-16} \left(\frac{T}{300}\right)^{-1.3} \exp\left(\frac{-23}{T}\right) \text{ cm}^3 \text{ s}^{-1}$ |
|-------------------------------------|---|
| $CH + O \longrightarrow CO + H$     | $k_{17} = 6.02 \times 10^{-11} \left(\frac{T}{300}\right)^{0.1} \exp\left(\frac{4.5}{T}\right) \text{ cm}^3 \text{ s}^{-1}$ |
| $CO + \gamma \longrightarrow C + O$ | $k_{18} = 1.35 \times 10^{-10}  \mathrm{s}^{-1}$  |
| $CH + \gamma \longrightarrow C + H$ | $k_{19} = 1.13 \times 10^{-9}  \mathrm{s}^{-1}$   |

#### **B.3** Balance equations of species

To distinguish between the hydrogen nuclei density  $n_{\rm H}$  and the number density of atomic hydrogen,  $n_{\rm HI}$  is used to denote the latter quantity. The ionisation fraction  $x_{\rm e}$  is defined as  $x_{\rm e} \equiv n_{\rm e}/n_{\rm H}$ . The first step is to express every species in the GL74 network in terms of  $n_{\rm H}$ ,  $f_{\rm H_2}$  and  $n_{\rm e}$ . The balance equations in GL74 network are:

For  $H_3^+$ :

$$k_{15}n_{\rm H_2}n_{\rm H_2^+} = (k_{12} + k_{13})n_{\rm e}n_{\rm H_3^+} \tag{B.1}$$

$$n_{\rm H_3^+} = \frac{k_{15}n_{\rm H}J_{\rm H_2}n_{\rm H_2^+}}{2k_{13}n_{\rm e}} \tag{B.2}$$

For  $H_2^+$ :

$$k_4 n_{\rm H_2} = n_{\rm H_2^+} (k_{14} n_{\rm H\,I} + k_{15} n_{\rm H_2} + k_{11} n_{\rm e}) \tag{B.3}$$

$$n_{\rm H_2^+} = \frac{k_4 n_{\rm H} f_{\rm H_2} / 2}{k_{14} n_{\rm H} + (k_{15} / 2 - k_{14}) f_{\rm H_2} n_{\rm H} + k_{11} n_{\rm e}} \tag{B.4}$$

For H<sub>2</sub>:

$$k_1 n_{\rm HI} n_{\rm H} + k_{14} n_{\rm HI} n_{\rm H_2^+} + k_{12} n_{\rm e} n_{\rm H_3^+} = \left[ (k_4 + k_5 + k_2) + k_{15} n_{\rm H_2^+} + k_{16} n_{\rm C^+} \right] n_{\rm H_2} \quad (B.5)$$

$$n_{\rm H_2} = \frac{k_1 n_{\rm H_1} n_{\rm H} + k_1 4 n_{\rm H_1} n_{\rm H_2^+} + k_{12} n_{\rm e} n_{\rm H_3^+}}{(k_4 + k_5 + k_2) n_{\rm H_2} + k_{15} n_{\rm H_2} n_{\rm H_2^+} + k_{16} n_{\rm H_2} n_{\rm C^+}}$$
(B.6)

$$\frac{f_{\rm H_2}}{2} = \frac{k_1(1-f_{\rm H_2})n_{\rm H} + k_{14}(1-f_{\rm H_2})n_{\rm H_2^+} + k_{12}x_{\rm e}n_{\rm H_3^+}}{(k_4+k_5+k_2) + k_{15}n_{\rm H_2^+} + k_{16}n_{\rm C^+}}$$
(B.7)

For H<sup>+</sup>:

$$k_3 n_{\rm H\,I} + k_{14} n_{\rm H_2^+} n_{\rm H\,I} = k_8 n_{\rm e} n_{\rm H^+} \tag{B.8}$$

$$n_{\rm H^+} = \frac{(k_3 + k_{14}n_{\rm H_2^+})n_{\rm H\,I}}{k_8 n_{\rm e}} \tag{B.9}$$

$$n_{\rm H^+} = \frac{(k_3 + k_{14}n_{\rm H_2^+})(1 - f_{\rm H_2})n_{\rm H}}{k_8 n_{\rm e}} \tag{B.10}$$

For He<sup>+</sup>:

$$k_6 n_{\rm He\,I} = k_9 n_{\rm e} n_{\rm He^+} \tag{B.11}$$

$$n_{\rm He^+} = \frac{(k_6/k_9 n_{\rm e}) x_{\rm He} n_{\rm H}}{1 + (k_6/k_9 n_{\rm e}) x_{\rm He} n_{\rm H}}$$
(B.12)

Here  $n_{\rm C}$  and  $n_{\rm CO}$  are found in terms of  $n_{\rm C^+}$  by using the total gas phase carbon abundance:

$$x_{\rm C,g} n_{\rm H} = n_{\rm C^+} + n_{\rm C} + n_{\rm CO} \tag{B.13}$$

$$x_{\rm C,g} = x_{\rm C^+} + x_{\rm C} + x_{\rm CO} \tag{B.14}$$

where  $x_{C,g}$  is the gas phase carbon abundance (number of carbon atoms in the gas phase per H).



FIGURE B.1: For reference, this is the chemical network of carboncontaining species

After adding in the new reactions, the balance equation for  $H_3^+$  is:

$$k_{15}n_{\rm H_2}n_{\rm H_2^+} = \left[ (k_{12} + k_{13})n_{\rm e} + k_{20}n_{\rm C} \right] n_{\rm H_3^+} \tag{B.15}$$

$$n_{\rm H_3^+} = \frac{k_{15} f_{\rm H_2} n_{\rm H} n_{\rm H_2^+}}{(k_{12} + k_{13}) n_{\rm e} + k_{20} n_{\rm C}}$$
(B.16)

#### **B.3.1** Balance equation for C

The balance equation for  $n_{\rm C}$  is:

$$\left(k_7 G_{\rm FUV} + k_{20} n_{\rm H_3^+}\right) n_{\rm C} = k_{10} n_{\rm e} n_{\rm C^+} + k_{16} n_{\rm C^+} n_{\rm H_2} \left(\frac{k_{19} G_{\rm FUV}}{k_{17} n_{\rm O} + k_{19} G_{\rm FUV}}\right)$$
(B.17)  
$$n_{\rm C} = \left(\frac{n_{\rm C^+}}{k_7 G_{\rm FUV} + k_{20} n_{\rm H_3^+}}\right) \left(k_{10} n_{\rm e} + \frac{k_{16} k_{19} f_{\rm H_2} n_{\rm H} G_{\rm FUV}}{2(k_{17} n_{\rm O} + k_{19} G_{\rm FUV})}\right)$$
(B.18)

Substitute Equation B.16 into B.18,

$$n_{\rm C} = n_{\rm C^+} \left( k_{10} n_{\rm e} + \frac{k_{16} k_{19} f_{\rm H_2} n_{\rm H} G_{\rm FUV}}{2(k_{17} n_{\rm O} + k_{19} G_{\rm FUV})} \right) \left( k_7 G_{\rm FUV} + \frac{k_{15} k_{20} f_{\rm H_2} n_{\rm H} n_{\rm H_2^+}}{(k_{12} + k_{13}) n_{\rm e} + k_{20} n_{\rm C}} \right)^{-1}$$
(B.19)

Let  $k_{C,1} = k_7 G_{FUV}$ ,  $k_{C,2} = (k_{12} + k_{13})n_e$ ,  $k_{C,3} = k_{15}k_{20}f_{H_2}n_Hn_{H_2^+}/2$  and  $k_{C,4} = k_{10}n_e + (k_{16}k_{19}f_{H_2}n_HG_{FUV})/(2(k_{17}n_O + k_{19}G_{FUV}))$ ,

$$n_{\rm C} = \left(k_{\rm C,1} + \frac{k_{\rm C,3}}{k_{\rm C,2} + k_{20}n_{\rm C}}\right)^{-1} k_{\rm C,4} n_{\rm C^+} \tag{B.20}$$

This equation can be rearranged to give:

$$\alpha_1 n_{\rm C}^2 + \alpha_2 n_{\rm C} + \alpha_3 = 0, \tag{B.21}$$

where

$$\alpha_1 = k_{\rm C,1} k_{20} \tag{B.22}$$

$$\alpha_2 = k_{\rm C,3} + k_{\rm C,1}k_{\rm C,2} - k_{20}k_{\rm C,4}n_{\rm C^+} \tag{B.23}$$

$$\alpha_3 = -k_{C,2}k_{C,4}n_{C^+} \tag{B.24}$$

#### **B.3.2** Balance equation for CO

The balance equation for CO is:

$$k_{18}G_{\rm FUV}n_{\rm CO} = k_{16}n_{\rm C^+}n_{\rm H_2}\frac{k_{17}n_{\rm O}}{k_{17}n_{\rm O} + k_{19}G_{\rm FUV}}$$
(B.25)

Since the only oxygen-containing species in the gas are O and CO, we can write

$$x_{\mathrm{O},\mathrm{g}}n_{\mathrm{H}} = n_{\mathrm{O}} + n_{\mathrm{CO}} \tag{B.26}$$

$$x_{\rm O,g} = x_{\rm O} + x_{\rm CO}$$
 (B.27)

CO forms from the reaction between CH and O, and CH can be formed from two pathways:

(i)  $C^+ + H_2 \longrightarrow CH_2^+ \dashrightarrow CH$ (ii)  $C + H_3^+ \dashrightarrow CH_2^+ \dashrightarrow CH$ 

CH and  $CH_2^+$  are assumed to be a transitory species, so their abundances are not checked in the chemical model.

The balance equation of CO is:

$$k_{18}G_{\rm FUV}n_{\rm CO} = (k_{16}n_{\rm C^+}n_{\rm H_2} + k_{20}n_{\rm C}n_{\rm H_3^+}) \frac{k_{17}(n_{\rm O,tot} - n_{\rm CO})}{k_{17}(n_{\rm O,tot} - n_{\rm CO}) + k_{19}G_{\rm FUV}}$$
(B.28)  
$$k_{17}k_{18}G_{\rm FUV}(n_{\rm O,tot}n_{\rm CO} - n_{\rm CO}^2) + k_{18}k_{19}G_{\rm FUV}^2n_{\rm CO} = (k_{16}n_{\rm C^+}n_{\rm H_2} + k_{20}n_{\rm C}n_{\rm H_3^+})(k_{17}n_{\rm O,tot} - k_{17}n_{\rm CO})$$
(B.29)

$$k_{18}G_{\rm FUV}(n_{\rm O,tot}n_{\rm CO} - n_{\rm CO}^2) + \frac{k_{18}k_{19}}{k_{17}}G_{\rm FUV}^2n_{\rm CO} = (k_{16}n_{\rm C^+}n_{\rm H_2} + k_{20}n_{\rm C}n_{\rm H_3^+})(n_{\rm O,tot} - n_{\rm CO})$$
(B.30)

Define  $k_{\text{CO},1} \equiv k_{18}G_{\text{FUV}}, k_{\text{CO},2} \equiv k_{18}k_{19}G_{\text{FUV}}^2/k_{17}, k_{\text{CO},3} \equiv k_{16}n_{\text{H}_2}n_{\text{C}^+},$ 

$$k_{\rm CO,1}(n_{\rm O,tot}n_{\rm CO} - n_{\rm CO}^2) + k_{\rm CO,2}n_{\rm CO} = (k_{\rm CO,3} + k_{20}n_{\rm C}n_{\rm H_3^+})(n_{\rm O,tot} - n_{\rm CO})$$
(B.31)

Here we use the relation

$$n_{\rm H_3^+} = \frac{k_{15}n_{\rm H_2}n_{\rm H_2^+}}{(k_{12} + k_{13})n_{\rm e} + k_{20}n_{\rm C}} \tag{B.32}$$

and define  $k_{\text{CO},4} \equiv k_{15} n_{\text{H}_2} n_{\text{H}_2^+}$  and  $k_{\text{CO},5} \equiv (k_{12} + k_{13}) n_{\text{e}}$ ,

$$n_{\rm H_3^+} = \frac{k_{\rm CO,4}}{k_{\rm CO,5} + k_{20}n_{\rm C}}.$$
(B.33)

Substituting Equation **B.33** into Equation **B.31**:

$$k_{\text{CO},1}(n_{\text{O,tot}} - n_{\text{CO}})n_{\text{CO}} + k_{\text{CO},2}n_{\text{CO}} = \left[k_{\text{CO},3} + k_{20}n_{\text{C}}\left(\frac{k_{\text{CO},4}}{k_{\text{CO},5} + k_{20}n_{\text{C}}}\right)\right](n_{\text{O,tot}} - n_{\text{CO}})$$
$$k_{\text{CO},1}n_{\text{CO}} + \frac{k_{\text{CO},2}n_{\text{CO}}}{n_{\text{O,tot}} - n_{\text{CO}}} = k_{\text{CO},3} + k_{20}n_{\text{C}}\left(\frac{k_{\text{CO},4}}{k_{\text{CO},5} + k_{20}n_{\text{C}}}\right)$$

Now we use  $n_{C,tot} = (1 - F_{gr,C})ZX_{C,\odot}n_H$  and  $n_C = n_{C,tot} - n_{C^+} - n_{CO}$  and define  $n_{C^*} = n_{C,tot} - n_{C^+}$ ,

$$k_{\text{CO},1}n_{\text{CO}} + \frac{k_{\text{CO},2}n_{\text{CO}}}{n_{\text{O},\text{tot}} - n_{\text{CO}}} = k_{\text{CO},3} + k_{20}(n_{\text{C}}^* - n_{\text{CO}}) \left(\frac{k_{\text{CO},4}}{k_{\text{CO},5} + k_{20}(n_{\text{C}}^* - n_{\text{CO}})}\right)$$
$$k_{\text{CO},1}k_{\text{CO},5}n_{\text{CO}} + k_{20}k_{\text{CO},1}(n_{\text{C}^*} - n_{\text{CO}}) + \frac{k_{\text{CO},2}n_{\text{CO}}}{n_{\text{O},\text{tot}} - n_{\text{CO}}}k_{\text{CO},5} + \frac{k_{\text{CO},2}n_{\text{CO}}}{n_{\text{O},\text{tot}} - n_{\text{CO}}}k_{20}(n_{\text{C}^*} - n_{\text{CO}})$$
$$= k_{\text{CO},3}k_{\text{CO},5} + k_{20}k_{\text{CO},3}(n_{\text{C}^*} - n_{\text{CO}}) + k_{20}k_{\text{CO},4}(n_{\text{C}^*} - n_{\text{CO}})$$

Let  $k_{\text{CO},6} \equiv k_{\text{CO},1}k_{\text{CO},5}$ ,  $k_{\text{CO},7} \equiv k_{20}k_{\text{CO},1}$ ,  $k_{\text{CO},8} \equiv k_{\text{CO},2}k_{\text{CO},5}$ ,  $k_{\text{CO},9} \equiv k_{\text{CO},3}k_{\text{CO},5}$ ,  $k_{\text{CO},10} \equiv k_{20}(k_{\text{CO},3} + k_{\text{CO},4})$ ,

$$k_{\text{CO},6}n_{\text{CO}} + k_{\text{CO},7}(n_{\text{C}^*} - n_{\text{CO}}) + \frac{k_{\text{CO},8}n_{\text{CO}}}{n_{\text{O},\text{tot}} - n_{\text{CO}}} + \frac{k_{20}k_{\text{CO},2}n_{\text{CO}}}{n_{\text{O},\text{tot}} - n_{\text{CO}}}(n_{\text{C}^*} - n_{\text{CO}})$$
$$= k_{\text{CO},9} + k_{\text{CO},10}(n_{\text{C}^*} - n_{\text{CO}})$$

 $k_{\rm CO,6} n_{\rm O,tot} n_{\rm CO} - k_{\rm CO,6} n_{\rm CO}^2 + k_{\rm CO,7} n_{\rm O,tot} (n_{\rm C^*} - n_{\rm CO}) n_{\rm CO} + k_{\rm CO,7} (n_{\rm C^*} - n_{\rm CO}) n_{\rm CO}^2$ 

 $+ k_{CO,8}n_{CO} + k_{20}k_{CO,2}(n_{C^*} - n_{CO})n_{CO}$ 

 $= k_{\rm CO,9} n_{\rm O,tot} - k_{\rm CO,9} n_{\rm CO} + k_{\rm CO,10} n_{\rm O,tot} (n_{\rm C^*} - n_{\rm CO}) - k_{\rm CO,10} (n_{\rm C^*} - n_{\rm CO}) n_{\rm CO}$ 

 $k_{\rm CO,6}n_{\rm O,tot}n_{\rm CO} - k_{\rm CO,6}n_{\rm CO}^2 + k_{\rm CO,7}n_{\rm O,tot}n_{\rm C^+}n_{\rm CO} - k_{\rm CO,7}n_{\rm C^+}n_{\rm CO}^2 + k_{\rm CO,7}n_{\rm CO}^3$ 

 $+ k_{\text{CO},8}n_{\text{CO}} + k_{20}k_{\text{CO},2}n_{\text{C}^*}n_{\text{CO}} - k_{20}k_{\text{CO},2}n_{\text{CO}}^2$ =  $k_{\text{CO},9}n_{\text{O},\text{tot}} - k_{\text{CO},9}n_{\text{CO}} + k_{\text{CO},10}n_{\text{O},\text{tot}}n_{\text{C}^*} - k_{\text{CO},10}n_{\text{O},\text{tot}}n_{\text{CO}} - k_{\text{CO},10}n_{\text{C}^*}n_{\text{CO}} + k_{\text{CO},10}n_{\text{CO}}^2$ 

This can be arranged into a cubic equation:

$$An_{\rm CO}^3 + Bn_{\rm CO}^2 + Cn_{\rm CO} + D = 0$$
(B.34)

where

$$A = k_{\rm CO,7},$$

 $B = -(k_{\rm CO,6} + k_{\rm CO,7}n_{\rm O,tot} + k_{\rm CO,7}n_{\rm C^*} + k_{20}k_{\rm CO,2} + k_{\rm CO,10}),$ 

- $C = k_{\text{CO},6} n_{\text{O},\text{tot}} + k_{\text{CO},7} n_{\text{O},\text{tot}} n_{\text{C}^*} + k_{\text{CO},8} + k_{20} k_{\text{CO},2} n_{\text{C}^*} + k_{\text{CO},9} + k_{\text{CO},10} n_{\text{O},\text{tot}} + k_{\text{CO},10} n_{\text{C}^*},$
- $D = -(k_{\text{CO},9}n_{\text{O,tot}} + k_{\text{CO},10}n_{\text{O,tot}}n_{\text{C}^*}).$

## Appendix C

## **Cosmic ray heating of** H<sub>2</sub>

#### C.1 Heating from elastic collisions and rotational excitation

 $Q_{\rm el/rot}$  can be expressed as

$$Q_{\rm el/rot}({\rm H}_2,{\rm e}) = \eta({\rm H}_2,{\rm e})W({\rm H}_2,{\rm e})$$
 (C.1)

 $W(H_2, e)$  is the energy required to produce a  $(H_2^+, e^-)$  pair and it is 74.6 eV for E = 30 eV.

 $\eta$ (H<sub>2</sub>, e) can be calculated similarly to  $\eta$ (HI, e) with Eqn.6 in Dalgarno, Yan, and Liu (1999) and the following constants:  $\eta_0 = 0.100$ ,  $\alpha = 0.515$ , C = 17.7. These constants are found in Table 7 of DYL99 if E = 30 eV in a H<sub>2</sub>-He mixture.

With  $x_e = 10^{-4}$ ,  $\eta(H_2, e) = 0.220$ ,  $Q_{el/rot} = 16.4$  eV. With  $x_e = 10^{-3}$ ,  $\eta(H_2, e) = 0.402$ ,  $Q_{el/rot} = 30.0$  eV.

#### **C.2** Heating from dissociation of H<sub>2</sub>

According to Table 5 in DYL99, for an electron energy *E* of 30 eV, there are 30/34.7 = 0.865 dissociations per electron. Adopting DYL's estimate of 5.4 eV per dissociation, the dissociation heating is 4.67 eV per electron, or 12.0 eV per ion pair. Now Equation 11 in GGP12 can be used to calculate the dissociation heating  $Q_{diss}$ :

$$Q_{\rm diss} = \frac{x({\rm H}_2)}{x({\rm H}) + x({\rm H}_2)} \frac{D_0}{1 + C x_{\rm e}^{\alpha}} \tag{C.2}$$

where  $D_0 = 12.0 \text{ eV}$ ,  $\alpha = 0.872$ , C = 17.7.

When f = 1 and  $x_e = 10^{-4}$ ,  $Q_{diss} = 11.93$  eV. When f = 1 and  $x_e = 10^{-3}$ ,  $Q_{diss} = 11.50$  eV.

#### C.3 Vibrational heating

As discussed in Section 3.3 of Glassgold, Galli, and Padovani (2012), after vibrational levels of H<sub>2</sub> is excited by fast electrons, the excitation energy goes into heating if the densities are high enough for the levels to be collisionally de-excited. If the  $n_{\rm H} < n_{\rm cr}$ , no heating from vibrational levels should be expected. As shown in Table 6 in GGP12, for a molecular cloud clump with  $n_{\rm H} = 10^4$  cm<sup>-3</sup>, the heating coming from vibrational levels  $Q_{\rm vib} = 0$  eV. Therefore, it can be assumed that  $Q_{\rm vib} = 0$  eV as long as the hydrogen density is not very high.

#### C.4 Chemical heating

The chemical heating due to formation of  $H_2^+$  is

$$Q_{\rm chem}({\rm H}_2^+) = \frac{x({\rm H}_2)}{x({\rm H}) + x({\rm H}_2)} F({\rm H}_2^+) P({\rm H}_2^+, {\rm H}_3^+) q_{\rm e}({\rm H}_2^+)$$
(C.3)

The branching ratio of  $H_2^+$  is  $F(H_2^+) = 0.88$ .

The probability that  $H_2^+$  turns into  $H_3^+$  (by reacting with  $H_2$  instead of  $e^-$ ), is

$$P(H_2^+, H_3^+) = \frac{kx(H_2)}{kx(H_2) + \beta x_e}$$
(C.4)

where  $\beta = 2.0 \times 10^{-7} T^{-1/2} \text{ cm}^{-3} \text{ s}^{-1}$ .

 $H_2^+$  can be destroyed by two pathways:

$$H_2^+ + e^- \longrightarrow 2H$$
 (C.5)

$$H_2^+ + H_2 \longrightarrow H_3^+ + H \tag{C.6}$$

with a combined rate coefficient of  $k = 2 \times 10^{-9} \text{ cm}^{-3} \text{ s}^{-1}$ .

 $H_3^+$  can be destroyed by dissociative recombination:

$$H_3^+ + e^- \longrightarrow H_2 + H \quad (25\%) \tag{C.7}$$

$$H_3^+ + e^- \longrightarrow 3H$$
 (75%) (C.8)

with a total rate coefficient of  $\beta' = 4.5 \times 10^{-6} T^{-0.65} \text{ cm}^3 \text{ s}^{-1}$ .

 $q_{\rm e}({\rm H}_2^+) = 7.6 \text{ eV}$  is the energy released in the recombination of  ${\rm H}_2^+$ . The chemical energy released by the formation of  ${\rm H}^+$  and  ${\rm He}^+$ , according to GGP12, are much less than the energy released by the formation of  ${\rm H}_2^+$ . Therefore, for the calculation of  $Q_{\rm chem}$ , I only consider the effects of  ${\rm H}_2^+$ .

 $Q(H_2)$  is mainly determined by f and  $x_e$ , and weakly by T. In addition, x(CO) and x(O) are required to calculate  $Q_{chem}$ .

### Appendix D

## Atomic physics of line emission

This section describes the atomic physics of line emission, using CO as an example. The process of calculating the Einstein A coefficient, Einstein B coefficient and collisional excitation coefficient are given below.

For a rigidly rotating diatomic molecule such as CO, the rotational energy levels are given by

$$E = hcB_{\rm rot}J(J+1) \tag{D.1}$$

where  $B_{\rm rot}$  is the rotational constant and *J* the rotational quantum number.

The relationship between the Einstein A and Einstein B coefficients is:

$$A_{\rm ul} = \frac{2h\nu_{\rm ul}^3}{c^2} B_{\rm ul} \tag{D.2}$$

where  $A_{ul}$  is the coefficient for spontaneous emission (with units of s<sup>-1</sup>) and  $B_{ul}$  is the coefficient for induced emission (with units of erg<sup>-1</sup> cm<sup>2</sup> s<sup>-1</sup> sr). The relationship between  $B_{ul}$  and  $B_{lu}$  is given by

$$g_{l}B_{lu} = g_{u}B_{ul} \tag{D.3}$$

where  $B_{lu}$  is the coefficient for induced absorption,  $g_l$  and  $g_u$  are the degeneracies for the lower and upper levels respectively. For a molecule like CO which has a permanent dipole,  $g_J = 2J + 1$ , where *J* is the total angular momentum of the rotational level.

The collisional excitation coefficients  $C_{lu}$  can be calculated from the collisional deexcitation coefficients using the following equation:

$$C_{\rm lu} = C_{\rm ul} \frac{g_{\rm u}}{g_{\rm l}} \,\mathrm{e}^{-E_{\rm ul}/kT} \tag{D.4}$$

where  $E_{ul}$  is the energy of the transition from the upper level to the lower level.

## Appendix E

# Draine & Sutin 1987's theory for collisional charging

Draine and Sutin (1987) (DS87) show an elaborate theory on the collisional charging of interstellar dust grains. For charged particles with charge  $q_i$ , mass  $m_i$ , number density  $n_i$  and sticking coefficient  $s_i$  arriving at the dust grains, if the charged particles have a Maxwellian distribution at infinity, they show that

$$J_i(Z) = n_i s_i \left(\frac{8k_{\rm B}T}{\pi m_i}\right)^{1/2} \pi a^2 \tilde{J}\left(\tau = \frac{ak_{\rm B}T}{q_i^2}, \xi = \frac{Ze}{q_i}\right)$$
(E.1)

where  $J_i$  is the rate at which charged particles arrive at the grain surface,  $\tau \equiv ak_{\rm B}T/q_i^2$  is the "reduced temperature", and

$$\tilde{J}(\tau,\xi) \equiv \int_0^\infty x \, \mathrm{e}^{-x} \, \tilde{\sigma}(\epsilon = x\tau,\xi) \, \mathrm{d}x. \tag{E.2}$$

where  $\tilde{\sigma}(\epsilon, \xi)$  is the "reduced cross-section", which takes the "image potential" into account, the electric potential resulting from the polarization of the grain induced by the Coulomb field of the incident charged particle. If  $\xi < 0$ ,  $\tilde{\sigma}$  decreases with increasing  $\epsilon \equiv Ea/q_i^2$ , where *E* is the kinetic energy (at infinity) of the charged particle. In other words, for a certain grain radius *a*, electrons with higher kinetic energy has a lower effective collisional cross-section with the grain due to image potential. x > 0 in Equation E.2 is the root of the equation is a root of the equation.

$$(2\epsilon x - \xi)(x^2 - 1)^2 - x = 0$$
(E.3)

For more details, see DS87.

DS87 helpfully supplies analytic approximations for  $\tilde{J}(\tau, \xi)$ :

$$\tilde{J}(\tau,\xi<0) \approx \left(1-\frac{\xi}{\tau}\right) \left[1+\left(\frac{2}{\tau-2\xi}\right)^{1/2}\right]$$
(E.4)

$$\tilde{J}(\tau,\xi=0) = 1 + \frac{\pi}{2\tau}^{1/2}$$
 (E.5)

$$\tilde{J}(\tau,\xi>0) \approx \left[1 + (4\tau + 3\xi)^{-1/2}\right]^2 e^{-\theta_{\xi}/\tau}$$
 (E.6)

where

$$\theta_{\xi} \approx \frac{\xi}{1 + \xi^{-1/2}}.\tag{E.7}$$

Using DS87's analytical expressions, it is possible to calculate the electron accretion rate  $J_e$  with acceptable accuracy.

## Appendix F

# Semi-analytical spherical cloud model

The model adopts a fixed radial distribution of density  $\rho(r)$  over radius r, according to a King profile of scale length l. This distribution is an approximate solution of the equation of hydrostatic support of an isothermal self-gravitating cloud with mass M and  $\rho_0 = \rho(0)$ :

$$\rho = \rho_0 \left[ 1 + \left(\frac{r}{l}\right)^2 \right]^{-3/2}, \tag{F.1}$$

$$l = \sqrt{\frac{kT}{4\pi G\rho_0 \mu m_{\rm H}}},\tag{F.2}$$

where *G* is Newton's gravitational constant and  $\mu$  is the mean molecular weight of the gas. One can write the mass enclosed within *r* as

$$M(r) = 4\pi\rho_0 l^3 f(\xi(r)),$$
(F.3)

$$f(\xi) = \frac{1}{2} \ln\left(\frac{1+\xi}{1-\xi}\right) - \xi, \tag{F.4}$$

$$\xi = \sin\left[\tan^{-1}\left(\frac{r}{l}\right)\right].\tag{F.5}$$

In this approximate treatment we relate *T* to a velocity dispersion *v* (an observable) at some  $r = r_v$ ;  $T = T_v$  with

$$\frac{3}{2}kT_v = \frac{1}{2}m_{\rm H}v^2 \longrightarrow kT_v = \frac{m_{\rm H}v^2}{3}$$
(F.6)

and at the radius  $r_v$ , relate  $M(r_v)$  with v using the virial theorem:

$$\frac{GM(r_v)m_{\rm H}}{r_v} = |{\rm PE}| = 2{\rm KE} = m_{\rm H}v^2,$$
(F.7)

$$M(r_v) = \frac{v^2 r_v}{G}.$$
(F.8)

It is convenient to define 3 radii in dimensionless form q = r/l with

$$q_l = 1$$
 for  $\underline{r} = l$ , with  $f(\xi(l)) = f(\xi_l)$  where  $\xi_l = 1/\sqrt{l}$ . (F.9)

$$q_v = \frac{r_v}{l} \text{ with } f(\xi(r_v)) = f(\xi_v).$$
(F.10)

$$q_{rt} = \frac{r_t}{l}$$
 (where  $r_t$  is the truncation radius) and  $f(\xi(r_t)) = f(\xi_{rt})$ . (F.11)

Then from Equation F.3 we can write for the total mass of the cloud,  $M_{\text{tot}}$ :

$$M_{\rm tot} = 4\pi\rho_0 l^3 f(\xi_{rt}), \tag{F.12}$$

$$M(r_v) = 4\pi \rho_0 l^3 f(\xi_v),$$
 (F.13)

$$M(l) = 4\pi\rho_0 l^3 f(\xi_l).$$
(F.14)

From Equation F.8 and Equation F.13:

$$4\pi\rho_0 l^3 f(\xi_v) = \frac{v^2 r_v}{G} = \frac{v^2 q_v l}{G},$$
 (F.15)

$$l = v \sqrt{\frac{q_v}{4\pi\rho_0 Gf(\xi_v)}}.$$
 (F.16)

From Equation F.2 and Equation F.4:

$$l^2 = \frac{v^2}{12\pi G\rho\mu}.\tag{F.17}$$

From Equation F.16 and Equation F.17:

$$f(\xi_v) = 3q_v\mu. \tag{F.18}$$

Solution of Equation F.15 defines the value of  $q_v = r_v/l$  to be used.

From Equation F.6,

$$kT_v = \frac{GM(r)m_{\rm H}}{3r_v},\tag{F.19}$$

and substitution for  $kT_v$  in Equation F.2, we obtain

$$l^{2} = \frac{GM(r)}{12\pi G\rho_{0}r_{v}\mu} = \frac{GM(r)}{12\pi G\rho_{0}q_{v}l\mu}$$
(F.20)

$$=\frac{M(r)}{12\pi\rho_0 q_v l\mu}.\tag{F.21}$$

$$l^{3} = \frac{M(r)}{12\pi\rho_{0}\mu q_{v}}.$$
 (F.22)

Since, from Equation F.12 and Equation F.8  $M(r) = M_{\text{tot}}\dot{f}(\xi_v)/f(\xi_{\text{rt}})$ , we can rewrite Equation F.22 as:

$$l^{3} = \frac{M_{\text{tot}}}{12\pi\rho_{0}\mu} \cdot \frac{f(\xi_{v})}{q_{v}f(\xi_{\text{rt}})}.$$
(F.23)

To solve for *l* and  $\rho_0$  one needs an independent value for  $\rho_0$ , which is derived by applying the external boundary conditions for the clump. These are given by  $\rho_{\text{ext}}$ ,  $T_{\text{ext}}$ , which is the solution for the density and temperature of the ISM outside the clump,

calculated by application of the ISM code for the input parameters  $P_{\text{ext}}$ ,  $Z_{\text{ext}}$ ,  $\zeta_{\text{CR}}$  (respectively the midplane pressure in the galaxy, the metallicity, and the CR ionisation rate per H at the galactocentric radius at which the clump is situated). Specifically, it is required that  $\rho_{\text{rt}} = \rho_{\text{ext}}(P_{\text{ext}}, Z_{\text{ext}}, \zeta_{\text{CR}})$ .

Substituting for  $\rho_{\rm rt} = \rho_{\rm ext}$  in (1), with  $q_{\rm rt} = r_t/l$ :

$$\rho_0 = \rho_{\text{ext}} (1 + q_{\text{rt}}^2)^{3/2}. \tag{F.24}$$

So from Equation F.23:

$$l = \left(\frac{M_{\text{tot}}}{12\pi\rho_{\text{ext}}\mu}\right)^{1/3} \left(\frac{f(\xi_v)}{q_v f(\xi_{\text{rt}})}\right)^{1/3} (1+q_{\text{rt}}^2)^{-1}.$$
 (F.25)

Equation F.25 completely specifies *l*, except for an unknown truncation radius, through the term  $q_{rt}$ . However  $q_{rt}$  can be solved for by again applying the virial theorem: From Equation F.6:

$$\frac{GM(r_v)m_{\rm H}}{3r_v} = \frac{m_{\rm H}v^2}{3}.$$
 (F.26)

From Equations F.12, F.13, F.14:

$$\frac{GM_{\text{tot}}}{v^2} = q_v l \frac{f(\xi_{\text{rt}})}{f(\xi_v)},\tag{F.27}$$

$$l = \frac{GM_{\text{tot}}}{v^2} \frac{f(\xi_v)}{q_v f(\xi_{\text{rt}})}.$$
(F.28)

Eliminating *l* between Equation F.25 and F.28 we can solve for  $q_{rt}$ , thus specifying the truncation radius just as a function of observables *v* and the boundary density  $\rho_{ext}$ :

$$\left(\frac{M_{\text{tot}}}{12\pi\rho_{\text{ext}}\mu}\right)^{1/3} \left(\frac{f(\xi_v)}{q_v f(\xi_{\text{rt}})}\right)^{1/3} \left(1+q_{\text{rt}}^2\right)^{-1/2} = \frac{GM_{\text{tot}}}{v^2} \frac{f(\xi_v)}{q_v f(\xi_{\text{rt}})},\tag{F.29}$$

$$\frac{f(\xi_{\rm rt})^{2/3}}{\left(1+q_{\rm rt}^2\right)^{1/2}} = \left(12\pi\rho_{\rm ext}\mu M_{\rm tot}^2 \cdot \frac{f^2(\xi_v)}{q_v^2}\right)^{1/3} \frac{G}{v^2}.$$
(F.30)

Thus then specifies  $\xi_{rt}$ , since  $f(\xi_v)$  and  $q_v$  are given by the solution of Equation F.18, and  $v^2$  is fixed observationally. Once we have solved for  $r_t$  in this way, we can then fix *l* through Equation F.25, and  $\rho_0$  through Equation F.24. Thus, *l*,  $\rho_0$  can be uniquely determined as a function of a single unknown variable  $M_{tot}$ .

## Appendix G

# Derivation of the total pressure in a galactic disc

For a preliminary estimate of the mid-plane gas pressure based on a physical interpretation of radiative transfer modelling parameters using a basic infinite thin stellar disk for the gravitational potential, the gravitational force of gas above the mid-plane is: (independent of z)

$$F_{\rm grav} = 2\pi G \Sigma_{\rm tot} \tag{G.1}$$

where  $\Sigma_{tot}$  is the total surface density (gas + stars). The total surface density is

$$\Sigma_{\text{tot}} = \Sigma_* + \Sigma_{\text{gas}}, \tag{G.2}$$

where  $\Sigma_*$  is the stellar surface density and  $\Sigma_{gas}$  is the gas surface density. Assuming  $\Sigma_* \gg \Sigma_{gas}$  and the virial theorem applies in the mid-plane:

$$E_{\rm pot} = -2 F_{\rm grav} \, z_{\rm gas} \, m. \tag{G.3}$$

Using the virial theorem  $E_{\rm kin} = -E_{\rm pot}/2$ ,

$$\frac{1}{2}mv^2 = F_{\text{grav}} z_{\text{gas}} m \tag{G.4}$$

$$v^2 = 2F_{\rm grav} \, z_{\rm gas} = 2\pi G \, \Sigma_{\rm tot} \, z_{\rm gas}, \tag{G.5}$$

where v is the velocity dispersion and m represents the mass of a parcel of gas. From the disc structure described in Dopita and Ryder (1994):

$$v^{2} = 2\pi G \Sigma_{\text{tot}} \left( \frac{z_{\text{gas}}^{2}}{z_{*} + z_{\text{gas}}} \right).$$
(G.6)

The gas component defining the pressure is taken to be the diffuse WIM, mixed in with WNM. It defines the external pressure of pressure-supported clouds:

$$P_{\rm ext} = n(z) \, k_{\rm B} T \tag{G.7}$$

In the WIM, *T* is set by a balance between photoionisation and recombination.

The density distribution of the WIM, assuming gravity is dominated by thin disk, is

$$n(z) = n_0 e^{-z/z_{\text{gas}}},$$
 (G.8)

where  $n_0$  is the gas density at the mid-plane and

$$z_{\rm gas} = \frac{k_{\rm B}T}{2\pi\,G\,\Sigma_{\rm tot}\,m}.\tag{G.9}$$

In the case of gas and stellar disks of finite thickness, the solution to the Poisson equation gives a *z*-density distribution of matter (van der Kruit and Searle (1981)):

$$n(z) = n_0 \operatorname{sech}^2\left(\frac{z}{z_{\text{scale}}}\right) \tag{G.10}$$

where  $z_{\text{scale}} = z_{\text{gas}}^2 / (z_* + z_{\text{gas}})$ .

The gas surface density is

$$\Sigma_{\rm gas} = 2m \, z_{\rm gas} \, n_0 = \frac{2mk_{\rm B}T}{2\pi \, G \, \Sigma_{\rm tot} \, m} \cdot n_0 \tag{G.11}$$

$$=\frac{n_0 k_{\rm B} T}{\pi G \,\Sigma_{\rm tot}}\tag{G.12}$$

The pressure at the mid-plane is

$$P_{\rm ext}(0) = n_0 k_{\rm B} T = \pi G \Sigma_{\rm gas} \Sigma_{\rm tot} \tag{G.13}$$

The pressure at height z above the galactic plane is

$$P_{\text{ext}}(z) = P_{\text{ext}}(0) \operatorname{sech}^2\left(\frac{z}{z_{\text{scale}}}\right)$$
 (G.14)

# List of publications

Mark T. Rushton, **Yu Fung Wong** and Richard J. Tuffs. "Radiative transfer modelling of photoelectric heating of gas in the nearby spiral galaxy NGC628" (in preparation)

**Yu Fung Wong** and Richard J. Tuffs. "Effects of spectral shape of radiation field on grain photoelectric heating in the interstellar medium" (in preparation)

Material in all of the publications mentioned above is used in this thesis.

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