Molecular cooling in the diffuse interstellar medium

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ABSTRACT
We use a simple one-zone model of the thermal and chemical evolution of interstellar gas to study whether molecular hydrogen (H₂) is ever an important coolant of the warm, diffuse interstellar medium (ISM). We demonstrate that at solar metallicity, H₂ cooling is unimportant and the thermal evolution of the ISM is dominated by metal line cooling. At metallicities below 0.1 Z⊙, however, metal line cooling of low density gas quickly becomes unimportant and H₂ can become the dominant coolant, even though its abundance in the gas remains small. We investigate the conditions required in order for H₂ to dominate, and show that it provides significant cooling only when the ratio of the interstellar radiation field strength to the gas density is small. Finally, we demonstrate that our results are insensitive to changes in the initial fractional ionization of the gas or to uncertainties in the nature of the dust present in the low-metallicity ISM.

Key words: galaxies: ISM – ISM: clouds – ISM: molecules – stars: formation

1 INTRODUCTION
Observations of star formation within the Milky Way and other nearby metal-rich galaxies show that the surface density of star formation correlates better with the surface density of molecular gas than with the total surface density or the surface density of atomic gas [Leroy et al. 2008; Bigiel et al. 2008; 2011; Schruba et al. 2011; also Shetty, Kelly & Bigiel 2013]. It is natural to assume that this correlation arises because the presence of molecular gas is a necessary prerequisite for star formation, but recent studies by Krumholz, Leroy & McKee (2011), Krumholz (2012) and Glover & Clark (2012a,b) have shown that this interpretation is incorrect. Numerical simulations of star formation in dense gas clouds have been used to demonstrate that the star formation rate in these clouds is largely insensitive to the composition of the gas. If molecule formation and molecular cooling are artificially suppressed, the predicted star formation rate that one obtains is very similar to that coming from models that include molecular cooling (Glover & Clark 2012a). These models suggest that the observed correlation between molecular gas and star formation comes about because the conditions that favour star formation also favour the formation of molecules. Furthermore, they predict that this correlation will break down at low metallicities (Glover & Clark 2012b; Krumholz 2012). However, these studies focussed on the thermal physics of individual gas clouds that were assumed to have already been assembled from the diffuse interstellar medium (ISM). They did not address the issue of whether molecular gas can play an important role at an earlier stage of the process, prior to, or during the assembly of, these dense, cold clouds.

This question has been examined to some extent by a few previous numerical studies. Jappsen et al. (2007) performed simulations of protogalaxy formation using a simplified chemical model that accounted for H₂ formation and destruction, as well as the ionization and recombination of C, O and Si, and showed that under these conditions, H₂ cooling dominates over metal line cooling at low densities (n ~ 1 cm⁻³ and below) for metallicities Z < 0.1 Z⊙. However, their study did not include the effects of a pre-existing background radiation field, which is arguably a reasonable approach when considering the formation of the earliest protogalaxies, but which is unlikely to be valid for low metallicity galaxies in the local Universe.

More recently, Gnedin & Kravtsov (2011) reported that in their galaxy formation simulations, H₂ cooling dominates over metal-line cooling at temperatures of a few thousand Kelvin and below for simulations with various different gas-phase metallicities and UV field strengths. However, the limited spatial resolution of their model means that they have to include a clumping factor into their H₂ formation rate in order to correct for unresolved small-scale density fluctuations. This correction factor is easy to justify within regions representing dense atomic or molecular clouds, which are dominated by turbulence and therefore have significant

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density substructure, but it is less obvious whether including a correction of this form is appropriate for regions corresponding to lower density, warm patches of the ISM, which are dominated by thermal motions and hence have much less turbulent substructure.

Another important recent study is that of Aykutalp & Spaans (2011). They performed a series of simulations of a small protogalaxy \((M_{\text{tot}} \sim 10^9 M_\odot)\) and explored the effects of varying the initial metallicity of the gas and the strength of the ambient radiation field. They found that at metallicity below \(10^{-2}\), their model protogalaxies were cooled primarily by \(H_2\) and that cooling in these low metallicity systems was very sensitive to the strength of the radiation field, being largely suppressed for field strengths \(G_0 > 0.01\) in units of the Habing (1968) field.

One drawback of all of these studies is that their computational cost limits the number of simulations that can be performed and makes it difficult to explore a wide parameter space of densities, metallicities etc. Their results suggest that there are situations in which \(H_2\) cooling is important in the low density ISM, but these simulations do not, by themselves, allow us to identify the full range of physical conditions for which this is the case. For this reason, it is useful to study the interplay between chemistry and thermodynamics in the low density ISM using simpler methods that do not have a large computational cost.

In this paper, we carry out such a study. We use a simple one-zone model of the ISM, in which the chemical and thermal evolution of gas that is initially hot and ionized is followed in detail, but where the gas density is held constant. With this setup, we can follow the evolution over long periods of time for minimal computational cost, allowing us to explore the behaviour of the gas for a wide range of different densities, metallicities and UV field strengths.

2 NUMERICAL APPROACH

Our aim is to establish the physical conditions in which gas that is initially in a warm, low-density state can cool significantly within a dynamical time, which we take to be a necessary prerequisite for the formation of molecular clouds and, ultimately, stars. In order to do this, we make use of a very simple one-zone model of the thermal and chemical evolution of the ISM. In this model, we keep the gas density fixed, and simply track the evolution of the gas and dust temperatures, as well as the chemical composition of the gas. We note that although gas that is able to cool will likely also increase its density – either by gravitational collapse or due to the effects of isobaric compression from surrounding warmer material – gas that is unable to cool is unlikely to change its density significantly unless perturbed by some external force. Our model is therefore well-suited to identifying which gas can cool and which cannot, but will provide an incomplete picture of the behaviour of gas that does manage to cool.

We model the chemical and thermal evolution of the gas in the ISM using a simplified chemical network coupled with a detailed atomic and molecular cooling function. Our chemical model is based on three main sources. We take our treatment of the collisional gas-phase chemistry of hydrogen, helium and deuterium from Clark et al. (2011), and our treatment of the collisional gas-phase chemistry of carbon, oxygen and silicon from Glover & Jappsen (2007). Rates for the key photochemical reactions (e.g. \(H^-\) photodetachment, \(H_2\) photodissociation) are taken from Glover et al. (2010). Our model tracks the abundances of atomic and ionized carbon, oxygen and silicon, but does not include the formation of molecules containing these elements (e.g. \(CO\), water). However, we do not expect this simplification to significantly affect our conclusions (Glover & Clark 2012a). We account for the formation of \(H_2\) on dust grains using the standard Hollenbach & McKee (1979) prescription, but do not include any other grain-surface chemistry in our model.

Heating in our model comes primarily from the photoelectric effect and cosmic ray heating, with additional minor contributions from effects such as \(H_2\) formation heating or ultraviolet pumping of excited vibrational states of \(H_2\). Cooling is provided by the electronic excitation of atomic H, He and He\(^+\), rotational and vibrational emission from \(H_2\) and HD, fine structure and metastable line emission from C, C\(^+\), O, Si and Si\(^+\), and thermal emission from dust. Metastable line emission represents a new addition to our cooling function and is treated using the data given in Table 9 of Hollenbach & McKee (1989).

The collisional rate coefficients that we adopt for the various chemical reactions in our model are for the most part the same as in Glover & Jappsen (2007) (for the metals) and Clark et al. (2011) (for the H, He and D chemistry), but in a few cases we have updated the values, in light of new experimental or theoretical data. For the associative detachment reaction

\[ H^- + H \rightarrow H_2 + e^- \]  

we now use the new rate coefficient measured by Kreckel et al. (2010) in place of the older value referenced in Clark et al. (2011). For the mutual neutralization reaction

\[ H^- + H^+ \rightarrow H + H, \]  

we use the rate coefficient given in Croft, Dickinson & Gadea (1999), which agrees well with recent theoretical (Stenrup, Larson & Elander 2009) and experimental (Urbain et al. 2012) determinations. We have also updated several of the rate coefficients used in our cooling function. To model the contribution to the \(H_2\) cooling rate made by \(H_2\)-proton collisions, we now make use of the excitation rates recently calculated by Honvault et al. (2011, 2012) for the transitions for which these are available, supplementing them with data from Gerlich (1994) and Križ (2002) for those transitions for which newer data is not available. The contribution of \(H_2\)-electron collisions is now modelled using the excitation rate coefficient data of van Yoon et al. (2008), in place of the much older data used in our previous treatment (see Glover & Abel 2008). Finally, in our treatment of fine structure cooling, we now use the rate data for \(H_2\) collisions computed by Abrahamsson, Krems & Dalgarno (2007) in place of the older values used in Glover & Jappsen (2007).

We consider gas that is initially warm \((T = 10000\, \text{K})\) and fully ionized, although in Section 3.3 below we discuss the effects of starting with a reduced level of ionization. We explore the influence of three main free parameters: the gas density, the metallicity, and the strength of the interstellar

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radiation field (ISRF). We can describe the gas density in terms of the number density of hydrogen nuclei $n$, which is related to the mass density by $\rho = 1.4n/m_p$, where $m_p$ is the proton mass, and we have assumed a 10:1 ratio of hydrogen to helium, as is appropriate for the local ISM. To parameterize the metallicity, we assume that at solar metallicity, the elemental abundances of C, O and Si relative to hydrogen are the same as those measured in the warm neutral medium (see e.g. Sembach et al. 2000). At other metallicities, we assume that the elemental abundances simply scale linearly with the total metallicity $Z$. We therefore have

$$x_{\text{C},\text{tot}} = 1.41 \times 10^{-4} \left( \frac{Z}{Z_\odot} \right),$$  \hspace{1cm} (3)$$

$$x_{\text{O},\text{tot}} = 3.16 \times 10^{-4} \left( \frac{Z}{Z_\odot} \right),$$  \hspace{1cm} (4)$$

$$x_{\text{Si},\text{tot}} = 1.51 \times 10^{-5} \left( \frac{Z}{Z_\odot} \right),$$  \hspace{1cm} (5)$$

where $x_{\text{C},\text{tot}}$, $x_{\text{O},\text{tot}}$, and $x_{\text{Si},\text{tot}}$ are the total fractional abundances of these three elements. We also assume in most of our models that the dust-to-gas ratio, $D$, scales linearly with metallicity, although in Section 3.3.2 below we report the results of runs in which we adopted a steeper dependence of $D$ on $Z$.

To model the interstellar radiation field, we adopt the spectral shape described in Draine (1978) in the ultraviolet, and that from Mathis, Mezger & Panagia (1983) at longer wavelengths. We assume that the shape of the spectrum does not change as we change the normalization, $G_0$, where setting $G_0 = 1$ gives us the original Draine and Mathis et al. normalizations. In some of our models, we include an approximate treatment of the effects of H$_2$ self-shielding. This is modelled using a self-shielding function based on the work of Draine & Bertoldi (1996), but modified according to the prescription in Wolcott-Green, Haiman & Bryan (2011) in order to more accurately represent the effects of self-shielding in warm gas. As input to the self-shielding function, we need to provide an H$_2$ column density. We compute this as $N_{\text{H}_2} = n_{\text{H}_2}L_{\text{ss}}$, where $n_{\text{H}_2}$ is the current H$_2$ number density and $L_{\text{ss}}$ is a characteristic self-shielding scale length. In our default set-up, we set $L_{\text{ss}} = 0$, so that there is no self-shielding. We explore the effects of adopting a non-zero value of $L_{\text{ss}}$ in Section 3.3.3.

We adopt a cosmic ray ionization rate for atomic hydrogen given by $\zeta_{\text{HI}} = 10^{-16}G_0$ s$^{-1}$. We include a dependence on $G_0$ to reflect the fact that the cosmic rays ionization rate and the UV photodissociation rate would both be expected to increase as the star formation rate increases. The ionization rates for our other chemical species (H$_2$, He, C, etc.) relative to $\zeta_{\text{HI}}$ are scaled as described in Glover & Jappsen (2007).

3 RESULTS

3.1 ISM cooling without H$_2$

We begin our study by examining to what extent the ISM can cool in the absence of H$_2$ cooling. To do this, we use the one-zone model described in the previous section to explore the thermal evolution of the gas for a wide range of different densities, $0.1 \leq n \leq 10^3$ cm$^{-3}$, and ISRF strengths, $10^{-4} < G_0 < 1.0$, at eight different metallicities: $\log (Z/Z_\odot) = 0.0, -1.0, -1.5, -2.0, -2.5, -3.0, -3.5$ and $-4.0$. For each value of Z, $G_0$ and $n$, we run the model for a single gravitational free-fall time, $t_{\text{ff}} = (3\pi/32Gn)^{1/2}$, and examine the temperature at the end of this time period. Our choice of the free-fall time here is motivated by the classic Rees-Ostriker criterion for dynamical fragmentation (Rees & Ostriker 1977). However, we have verified that our results are not significantly different if we allow the gas to evolve for e.g. two free-fall times. Our results are plotted in Figure 1.

At solar metallicity, we see that there are two main temperature regimes. For values of $G_0/n$ greater than around 0.3, the gas remains hot, with a temperature of around 8000–9000 K. For lower values of $G_0/n$, however, the gas cools significantly, reaching temperatures of order a few hundred K when $G_0/n \sim 0.3$, and temperatures as low as 20 K when $G_0/n \leq 0.3$. We can understand this behaviour as a consequence of the fact that over a wide range in temperatures, the cooling of the neutral ISM is dominated by fine structure line emission, while the heating is dominated by photoelectric heating (see e.g. Wolfire et al. 1995, 2003). If we write the cooling rate as

$$\Lambda_{\text{cool}} = \Lambda_0(T) \left( \frac{Z}{Z_\odot} \right)^2,$$

where $\Lambda_0$ depends only weakly on $T$ for $T > 100$ K, and the heating rate as

$$\Gamma_{\text{pe}} = \Gamma_{0}(n_e,T) \frac{D}{D_{\text{ss}}} G_0 n,$$

where $\Gamma_0$ is also a weak function of $T$, then it is easy to show that in solar metallicity gas,

$$\frac{\Gamma_{\text{pe}}}{\Lambda_{\text{cool}}} \propto \frac{G_0}{\Lambda_0} \propto \frac{G_0}{n}.$$  \hspace{1cm} (8)$$

Since the temperature dependence of both the photoelectric heating rate and the fine structure cooling rate is weak in the temperature range of interest, it is the size of the factor $G_0/n$ that primarily determines whether heating or cooling dominates, and hence whether the gas remains close to its starting temperature, or cools until it reaches a temperature at which further fine structure cooling becomes ineffective.

If we now decrease the metallicity of the gas by an order of magnitude, we see that the main change which occurs is a slight increase in the size of the region in which cooling is significant, the critical value of $G_0/n$ decreases from 0.3 to around 0.1, but the behaviour of the gas for $G_0/n \ll 0.1$ or $G_0/n \gg 0.1$ does not significantly change. Again, this can be understood as a consequence of the cooling rate being dominated by fine structure emission and the heating rate by photoelectric emission from dust. Since we have assumed that the dust-to-gas ratio is proportional to the metallicity, both the heating and the cooling rates scale linearly with the metallicity, and the resulting equilibrium temperature is largely independent of metallicity. The fact that it is not completely independent is largely due to the fact that the cosmic ray heating rate does not decrease when the metallicity decreases, meaning that cosmic ray heating becomes increasingly dominant as we move to lower metallicities.

If we decrease the metallicity further, to $Z = 10^{-1.5}Z_\odot$, we find that there is a qualitative change in the behaviour.
of the gas. At densities \( n > 3 \text{ cm}^{-3} \), the gas behaves largely as before, but at lower densities, the gas remains warm regardless of the value of \( G_0 \). This change in behaviour is not due to a change in the equilibrium temperature of the gas, which remains low when \( G_0 \) is low. Instead, it reflects the fact that at low densities in this simulation, the gas does not have time to reach its equilibrium temperature. In this regime, the cooling time

\[
t_{\text{cool}} = \frac{1}{\gamma - 1} \frac{\rho_{\text{tot}} kT}{A},
\]

becomes larger than the free-fall time \( t_{\text{ff}} \) before the temperature of the gas can reach equilibrium. For example, consider the case of gas with \( T = 6000 \text{ K} \) at a number density \( n = 0.1 \text{ cm}^{-3} \). For these conditions, and for \( Z = 10^{-1.5} \text{ Z}_\odot \), the total cooling rate due to fine structure emission from C\(^+\), Si\(^+\) and O is approximately \( \Lambda_{\text{tot}} \approx 9.4 \times 10^{-30} \text{ erg s}^{-1} \text{ cm}^{-3} \). The cooling time of this gas is therefore at least \( 1.3 \times 10^{16} \text{ s} \), regardless of the value of \( G_0 \). This is significantly longer than the free-fall time, which for gas at this density is approximately \( t_{\text{ff}} \approx 4 \times 10^{15} \text{ s} \), and hence the gas is unable to cool below around 6000 K within a free-fall time.

Continuing to decrease the metallicity beyond this point makes it even harder for the gas to cool within a free-fall time, as its cooling time scales inversely with metallicity while its free-fall time remains fixed. By the time we reach a metallicity of \( Z = 10^{-3} \text{ Z}_\odot \), we see that none of the gas in the region of \( G_0 - n \) parameter space examined here can cool very much within a free-fall time.

It is also easy to see how these results would change if we examined the gas after a longer period of time. Since the limiting factor in the gas with low density and low \( G_0 \) is the time available for cooling, increasing the time period considered from \( t_{\text{ff}} \) to e.g. \( 2t_{\text{ff}} \) would shift the density at which the transition from hot gas to cold gas occurs, in this case by a factor of 4. Our precise results therefore depend on our choice of \( t_{\text{ff}} \) as the moment to examine the gas temperature. However, to completely offset the effects of a substantial drop in metallicity, one would have to consider a much longer time period; for example, a decrease in \( \text{Z}_\odot \) by a factor of ten could be mitigated by looking at the gas after ten free-fall times. In practice, it is unlikely that the gas would remain in an undisturbed state for such a long time period, and even if it did so, gas which can cool and collapse only on a timescale \( t \gg t_{\text{cool}} \) is unlikely to form stars efficiently.

In summary, we see that for the majority of the metallicities considered here, the main factor that limits the temperature to which the gas can cool within a free-fall time is not the influence of photoelectric and/or cosmic ray heating, it is simply the fact that the cooling time is long compared to the free-fall time.

### 3.2 ISM cooling with \( \text{H}_2 \)

We next look at how the ability of the ISM to cool changes once we include the effects of \( \text{H}_2 \) and HD cooling. In Figure 2, we show the results of a similar set of simulations to those in the previous section. The only difference in these simulations is that in this case, we account for molecular cooling. We see immediately that at solar metallicity, there is essentially no difference in the outcome. Indeed, if we quantitatively compare the temperatures reached at each point in \( G_0 \)-density space in this run with those in the model without \( \text{H}_2 \) cooling, we find that the maximum difference in the final temperature is less than 1%. We have also looked in detail at the fraction of the total cooling provided by \( \text{H}_2 \) throughout the lifetime of each of the runs, and find that this is never greater than around 10%. We can therefore immediately conclude that in metal-rich gas, and in the absence of self-shielding, \( \text{H}_2 \) cooling does not play a significant role in regulating the temperature. This is consistent with the idea that in galaxies like our own Milky Way, the observed correlation between molecular gas and star formation is a consequence of the fact that both molecules and stars form preferentially in regions with high column density and high volume density, rather than an indication that molecular cooling is required for star formation (see e.g. Krumholz, Leroy & McKee 2011; Glover & Clark 2012a,b; Krumholz 2012).

At lower metallicities, however, we start to see significant differences between the two sets of runs. We have already seen that in the runs without molecular cooling, as we lower the metallicity, the the question of whether a given parcel of gas can cool within a free-fall time becomes determined almost entirely by the gas density, with \( G_0 \) having little or no influence on whether the gas can cool. This is not the case in the runs that include molecular cooling. In these runs, \( G_0 \) plays an important role in determining the outcome of the simulations for all of the metallicities that we examine. For metallicities in the range \( 10^{-1.5} > Z > 10^{-2.5} \text{ Z}_\odot \), the boundary dividing those regions in \( G_0 \)-density space that cool from those that do not roughly follows a line along which \( G_0/n^{3/2} \) is constant, while at lower metallicities, the dividing line is better described as a line of constant \( G_0/n \). We see also that the temperature reached by the cooling gas increases significantly as we decrease the metallicity, from \( T \sim 10–20 \text{ K} \) at solar metallicity to \( T \sim 200–300 \text{ K} \) at \( 10^{-4} \text{ Z}_\odot \), although we caution that these numbers should be treated with care, as in a realistic system, it is likely that the gas would not remain at constant density as it cools. The difference between the runs with and without molecular cooling is particularly apparent at metallicities below \( 10^{-2} \text{ Z}_\odot \). At these metallicities, little cooling occurs in the runs without \( \text{H}_2 \), whereas in the runs with \( \text{H}_2 \), cooling remains efficient over a large portion of the parameter space that we examine.

In order to understand the behaviour that we find in these runs, and in particular why we recover the scalings that we do, it is useful to look at how the fractional abundance of \( \text{H}_2 \) evolves with time in gas. At metallicities \( Z > 0.01 \text{ Z}_\odot \), the final \( \text{H}_2 \) fraction is set by the balance between \( \text{H}_2 \) formation on dust and \( \text{H}_2 \) photodissociation (Glover 2003). We can write the \( \text{H}_2 \) formation rate as

\[
R_{\text{form}} = k_{\text{form}} n n_{\text{H}} \text{,}
\]

where \( k_{\text{form}} \) is the reaction rate coefficient for \( \text{H}_2 \) formation on grain surfaces (see e.g. Hollenbach & McKee 1977; Cazaux & Spaans 2004), \( n \) is the number density of hydrogen nuclei and \( n_{\text{H}} \) is the number density of atomic hydrogen. For the \( \text{H}_2 \) photodissociation rate, we have

\[
R_{\text{dis}} = k_{\text{dis}} n_{\text{H}} \text{,}
\]

where \( k_{\text{dis}} \) is the photodissociation rate per \( \text{H}_2 \) molecule, which for our adopted radiation field is given by \( k_{\text{dis}} = \ldots \)
Figure 1. Gas temperature at $t = t_{\text{ff}}$, computed as a function of the number density of hydrogen nuclei, $n$, and the strength of the interstellar radiation field in units of the standard value, $G_0$, for a set of runs covering a range of metallicities between $Z = Z_\odot$ and $Z = 10^{-4} Z_\odot$. In these runs, the effects of $\text{H}_2$ and HD cooling were not included.
Figure 2. As Figure 1, but for a set of runs that included the effects of H$_2$ and HD cooling.
5.6 \times 10^{-11} \text{cm}^3 \text{s}^{-1}. Combining these equations, it is easy to show that in chemical equilibrium, the H$_2$ number density is simply

$$n_{\text{H}_2, \text{eq}} = \frac{k_{\text{form}}}{k_{\text{dis}}} n n_H \propto G_0^{-1} n^2.$$

(12)

This equilibrium state is reached on a timescale $t_{\text{dis}} = k_{\text{dis}}^{-1} \simeq 1.8 \times 10^{10} G_0^{-1} \text{ s}$, and hence $t_{\text{dis}} \ll t_{\text{ff}}$ for the majority of the densities and UV field strengths that we examine. At densities far below the H$_2$ critical density $n_{\text{crit}} \sim 10^3 \text{cm}^{-3}$, the cooling time of the gas due to H$_2$ line cooling can be written as

$$t_{\text{cool}} \propto \frac{n T}{\Lambda_{\text{H}_2} n n_{\text{H}_2}}.$$

(13)

where $\Lambda_{\text{H}_2}$ is the H$_2$ cooling rate expressed in units of cm$^3$ s$^{-1}$, which is in general a strong function of temperature. At a fixed gas temperature, $t_{\text{cool}}$ therefore scales with the H$_2$ number density as

$$t_{\text{cool}} \propto n_{\text{H}_2}^{-1},$$

(14)

If we now set $t_{\text{cool}} = t_{\text{ff}}$, then since $t_{\text{ff}} \propto n^{-1/2}$, it is easy to demonstrate that our required H$_2$ number density varies as

$$n_{\text{H}_2, \text{req}} \propto n^{1/2}$$

(15)

as we change $n$. Comparing this with Equation (12) we see that if for some combination of $n$ and $G_0$ we have $n_{\text{H}_2, \text{eq}} = n_{\text{H}_2, \text{req}}$ (i.e. our equilibrium H$_2$ fraction is just enough to cool the gas within a free-fall time), then the same condition will hold for other values of $G_0$ and $n$ only if

$$G_0^{3/2} \simeq \text{constant},$$

(16)

in agreement with the behaviour that we see in Figure 2.

Below $Z \sim 0.01 Z_\odot$, the behaviour of the gas changes, owing to the increasing influence of the gas-phase processes

$$H + e^- \rightarrow H^- + \gamma,$$

(17)

$H^+$ and $H^-$ are the cooling time of the gas due to $H^+$ and $H^-$, respectively. At a fixed gas temperature, $n_{\text{H}_2}$ densities far below the $H^+$ and $H^-$, we have $n_{\text{H}_2, \text{req}} \propto n^{-1}$, which is in general a strong function of temperature. At a fixed temperature, $t_{\text{cool}}$ therefore scales with the H$_2$ number density as

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Below $Z \sim 0.01 Z_\odot$, the behaviour of the gas changes, owing to the increasing influence of the gas-phase processes

$$H + e^- \rightarrow H^- + \gamma,$$

(17)
the decreasing ionization also leads to a decreasing cooling rate per H$_2$ molecule, implies that most of the cooling that occurs in this case takes place at early times, prior to or at the point at which the H$_2$ abundance reaches its peak value. Consequently, the important timescale in this case is not the free-fall time, but rather is the time taken for the H$_2$ abundance to reach a maximum, which is simply the photodissociation time $t_{\text{dis}}$. If $t_{\text{cool}} \ll t_{\text{dis}}$, then the gas will cool, but if $t_{\text{cool}} \gg t_{\text{dis}}$, it will remain warm. As before, we know that

$$t_{\text{cool}} \propto n_{\text{H}_2}^{-1},$$

(22)

and it is also easy to show that the photodissociation time scales as

$$t_{\text{dis}} \propto \frac{1}{G_0},$$

(23)

independent of the value of the H$_2$ abundance. Therefore, the condition that $t_{\text{cool}} = t_{\text{dis}}$ implies that

$$\frac{G_0}{n_{\text{H}_2,\text{eq}}} = \text{constant},$$

(24)

where $n_{\text{H}_2,\text{eq}}$ is the equilibrium H$_2$ abundance. When $G_0/n$ is large, this scales with $n$ and $G_0$ as

$$n_{\text{H}_2,\text{eq}} = \frac{n^3}{G_0},$$

(25)

and hence our condition that $t_{\text{cool}} = t_{\text{dis}}$ is implies that

$$\frac{G_0}{n^3} = \text{constant},$$

(26)

and hence that

$$\frac{G_0}{n} = \text{constant},$$

(27)

in agreement with our simulation results.

3.3 Varying the model parameters

3.3.1 Initial ionization

So far, we have assumed, for simplicity, that the gas is initially fully ionized. However, we know that in practice this is an overestimate, as the typical ionization fraction in the warm neutral medium is closer to $x \sim 0.03$ (Wolfire et al. 1995). It is therefore important to establish whether this simplification significantly affects our results. We have therefore run a series of models that include both metal and H$_2$ cooling, but that start with fractional ionizations given by the following expression

$$x_0 = \min \left[ 1, 0.02n^{-1/2} \left( \frac{\zeta}{10^{-16} \text{ s}^{-1}} \right)^{1/2} \right],$$

(28)

where $\zeta$ is the cosmic ray ionization rate of atomic hydrogen. This expression yields values for $x_0$ that are close to the equilibrium value that we would obtain if cosmic ray ionization and radiative recombination were the only processes acting to change the ionization state of the gas.

We find that in general, the change in the initial ionization fraction has only a minor effect on the ability of the gas to cool. As an example, we show in Figure 4 the results that we obtain for a run with $Z = 10^{-3}Z_\odot$ and a low initial fractional ionization. If we compare this with the corresponding panel in Figure 2, we see that there are only a few differences – the region that is unable to cool has become slightly larger, and the final temperature reached by gas with high and low $G_0$ is also somewhat larger, but on the whole, the behaviour is very similar to that in the high ionization fraction case.

In the regions of parameter space dominated by metal-line cooling, it is easy to understand why changing the initial fractional ionization has so little effect. In these simulations, the cooling rate is sensitive to the fractional ionization only when the latter is very large (Dalgarno & McCray 1972). Therefore, although the cooling rate in the high ionization simulations is initially larger than that in the low ionization simulations, the cooling rates converge as the gas recombines and $x$ falls towards its equilibrium value.

It is slightly more surprising that changing $x_0$ has such a limited effect in the case where H$_2$ cooling dominates, since as we have seen, the H$_2$ formation rate in these runs depends on the fractional ionization. However, in practice, the dependence of the H$_2$ formation rate on $x$ becomes quite weak for $x > 0.03$, owing to the influence of the mutual neutralization reaction

$$\text{H}^- + \text{H}^+ \rightarrow \text{H} + \text{H}.$$  

(29)

When $x$ is large, most of the H$^-$ ions formed by reaction 17 are destroyed by this reaction and do not survive for long enough to form H$_2$. Consequently, within this regime, further increasing $x$ has only a minor effect on the H$_2$ formation rate and the peak H$_2$ abundance. For this reason, the effect that decreasing $x_0$ has on the peak H$_2$ abundance is much smaller than one might initially expect, thereby explaining why this change has only a limited effect on the ability of the gas to cool.

3.3.2 Dust-to-gas ratio

In most of our models, we assume that the dust-to-gas ratio, $D$, scales linearly with metallicity. This appears to be a good assumption for galaxies with metallicities close to that of the Milky Way (Sandstrom et al. 2012). However,
there are observational indications that at metallicities below around 0.3 \( Z_\odot \), \( D \) falls off more rapidly with decreasing metallicity than predicted by a simple linear scaling (Galametz et al. 2011; Herrera-Camus et al. 2012). We have therefore examined the effect of adopting a scaling for \( D \) that better matches the observational data, namely

\[
D = \begin{cases} \frac{D_\odot (Z/Z_\odot)}{0.3} & Z \geq 0.3 Z_\odot \\ 0.3 \frac{D_\odot (Z/Z_\odot)^2}{Z < 0.3 Z_\odot} \end{cases}
\]  

(30)

We find that changing the dust scaling in this fashion has little effect on our results. Obviously, for metallicities \( Z \geq 0.3 Z_\odot \), there is no change in \( D \) from the values used with our default set-up, and hence no change in behaviour. If we drop the metallicity to \( Z = 0.1 Z_\odot \), we do see a slight change in behaviour, as illustrated in Figure 5 the gas in the simulation with less dust cools more readily than the gas in the simulation with more dust. This is a consequence of the fact that photoelectric heating is still an important heat source in the diffuse ISM at these metallicities. By reducing the dust abundance, we reduce the photoelectric heating rate, making it easier for the gas to cool. Nevertheless, the difference between the two runs is small, and grows smaller still if we further reduce the metallicity. We can therefore be confident that the main results of this study are robust against uncertainties in the nature of the dust in low metallicity galaxies.

3.3.3 \( \text{H}_2 \) self-shielding

Up to this point, we have neglected the effects of \( \text{H}_2 \) self-shielding. However, it is not immediately obvious that this is a good approximation. The \( \text{H}_2 \) fractions that we find in the diffuse gas are small, but even \( \text{H}_2 \)-poor gas can produce a significant amount of self-shielding if its total column density is large enough. In the real ISM, the amount of self-shielding that we have at any given point depends on the distribution of \( \text{H}_2 \) column densities around that point, as well as the velocity field of the gas. Our simple one-zone model does not allow us to accurately account for these effects, and so to investigate the influence of self-shielding we instead adopt the approximation discussed in Section 2, we assume that the \( \text{H}_2 \) column density is directly related to the \( \text{H}_2 \) number density via

\[
N_{\text{H}_2} = n_{\text{H}_2} L_{\text{ss}}.
\]

In Figure 6 we show the results we obtain from a set of runs performed using this approximation, with \( L_{\text{ss}} = 10 \) pc.

Comparing the results plotted in Figures 2 and 6, we see that at metallicities \( Z \geq 10^{-1.5} Z_\odot \), the inclusion of \( \text{H}_2 \) self-shielding has little effect on the final gas temperature. In these simulations, the regions in \( G_0 \)-density parameter space where cooling is inefficient also correspond to regions where the peak \( \text{H}_2 \) fraction is very small. The \( \text{H}_2 \) column density in these regions therefore never becomes large enough to produce significant self-shielding of \( \text{H}_2 \), and the final result is therefore the same in simulations with and without this effect included. At higher densities and lower values of \( G_0 \), the peak \( \text{H}_2 \) fraction is much higher and the gas does become able to self-shield, but this occurs in regions that can already cool efficiently, and so once again the inclusion of \( \text{H}_2 \) self-shielding has little effect on the outcome. The only significant difference between the two sets of runs is in the minimum temperature reached by the gas with high density and low \( G_0 \): the inclusion of \( \text{H}_2 \) self-shielding allows this gas to cool to slightly lower temperatures than before. However, we caution that this result should be treated with caution as it is likely that in reality this strongly cooling gas will change its density in response to the loss of thermal support, rather than remaining at constant density as assumed in our model.

In the lower metallicity runs, \( Z < 10^{-2} Z_\odot \), the inclusion of \( \text{H}_2 \) self-shielding has a more pronounced effect. The boundary in \( G_0 \)-density space between regions that can and cannot cool becomes much sharper and also slightly steeper, corresponding to a line where \( G_0/n^{1/3} \sim \text{constant} \), rather than to a line of constant \( G_0/n \) as in the runs without self-shielding. The fact that the transition becomes sharper is easy to understand: it is simply a consequence of the sudden jump in the equilibrium abundance of \( \text{H}_2 \) that occurs once the gas becomes able to self-shield. This jump occurs because the onset of self-shielding leads to a drop in the photodissociation rate, which leads to an increase in the equilibrium \( \text{H}_2 \) abundance, which leads to an increase in the \( \text{H}_2 \) column density and hence a further drop in the photodissociation rate, etc. This positive feedback drives the equilibrium \( \text{H}_2 \) abundance sharply upwards once we enter the self-shielding regime.

The steepening of the transition is a consequence of the fact that by including self-shielding, we are including another source of density dependence: the amount by which self-shielding reduces the \( \text{H}_2 \) photodissociation rate depends on \( \text{n}_{\text{H}_2} \), which in turn depends on the density via Equation 31. Therefore, in gas with any given value of \( G_0/n \), self-shielding, and hence \( \text{H}_2 \) cooling, will always be more effective at large \( n \) (and hence large \( G_0 \)) than at small \( n \).

We have also examined the effect of varying \( L_{\text{ss}} \). We find, as one might expect, that decreasing \( L_{\text{ss}} \) leads to an increase in the size of the region that does not cool, whereas increasing \( L_{\text{ss}} \) has the opposite effect. However, in both cases the effect is fairly small. The reason for this is that \( n_{\text{H}_2} \) varies strongly as a function of \( G_0 \) and \( n \), as we have already seen, and hence the value of \( N_{\text{H}_2} \) at a given point in \( G_0 \)-density space depends far more on the value of \( n_{\text{H}_2} \) than on the value of \( L_{\text{ss}} \). Our main results are therefore robust against changes in \( L_{\text{ss}} \).

4 DISCUSSION

At first sight, it might appear that our results are in conflict with previous studies of star formation in metal-poor systems that typically find that metal-line cooling dominates over \( \text{H}_2 \) cooling at metallicities above a critical value of around \( 10^{-3.5} Z_\odot \) (see e.g. Bromm et al. 2001; Bromm & Loeb 2003; Frebel, Johnson & Bromm 2007; Smith et al. 2009), and that dust cooling can dominate at even lower metallicities (Schneider et al. 2002; Omukai et al. 2005; Clark, Glover & Klessen 2008). However, these studies were primarily concerned with higher density gas than is treated in this paper. For example, Frebel, Johnson & Bromm (2007) derive their constraints on the metallicity required to provide effective fine-structure

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cooling by considering the behaviour of gas at a density of $10^5 \text{ cm}^{-3}$ and a temperature of 200 K without addressing how the gas gets to this density and temperature in the first place. Similarly, studies of dust cooling in very metal-poor systems find that dust dominates the cooling only at very high densities (Dopcke et al. 2011, 2013).

In order to reach the densities at which metal cooling begins to dominate in these metal-poor systems, which are orders of magnitude higher than typical ISM densities, some other form of cooling is required. On possibility is Lyman-α cooling from atomic hydrogen, but this maintains the gas temperature at close to $10^4$ K, resulting in a very large Jeans mass ($M_J \sim 2 \times 10^7 n^{-1/2} M_\odot$). This will therefore be an important process only in relatively massive systems, such as protogalaxies illuminated by strong UV radiation fields (see e.g. Omukai, Schneider & Haiman 2008). What our results demonstrate is that when the ambient radiation field is relatively weak, molecular hydrogen alone can cool the gas in less than a free-fall time, thereby enabling it to collapse to the higher densities required for efficient metal cooling.

It is also interesting to compare our results for solar metallicity gas with those presented by Gnedin & Kravtsov (2011). In their simulations, Gnedin & Kravtsov (2011) find that the H$_2$ cooling rate is almost an order of magnitude larger than the metal-line cooling rate at temperatures of around 1000 K, and hence conclude that H$_2$ dominates the thermal evolution of the warm gas. On the other hand, in our solar metallicity simulations, we find that H$_2$ never provides more than about 10% of the total cooling, even in runs in which we account for the effects of H$_2$ self-shielding. The reason for this discrepancy is not entirely clear. Our treatment of H$_2$ cooling differs from that in Gnedin & Kravtsov (2011) owing to the changes we have made to our treatment of H$_2$-proton and H$_2$-electron collisions (see Section 2), but the overall change is at most a factor of three, far too little to account for the difference in our results. Gnedin & Kravtsov also make use of a different treatment of metal-line cooling, based on Penston (1970) and Dalgarno & McCray (1972), but do not provide enough information on the ionization state of the gas in their models to allow us to judge how significantly their total metal-line cooling rate differs from ours.

Finally, it is possible that the initial conditions that we adopt for the warm gas in our present study do not properly reflect the conditions that Gnedin & Kravtsov (2011) find in their 3D hydrodynamical simulation. Specifically, we assume that the gas is initially completely devoid of H$_2$. This means that the amount of H$_2$ available to participate in the cooling cannot be larger than the amount that can form within a cooling time, even if the equilibrium H$_2$ abundance is in principle much larger. In the Gnedin & Kravtsov (2011) simulations, some of their warm gas will have previously been cold, dense gas, and it may therefore retain some of the H$_2$ that it formed during this period. If so, then this would naturally lead to higher H$_2$ cooling rates than we find in our simulations.

5 SUMMARY

Our results demonstrate that H$_2$ cooling can potentially play an important role in regulating the temperature of the diffuse ISM, but only if two important conditions are met. First, the metallicity must be below 0.1 Z$_\odot$, as at higher metallicities, metal line cooling dominates throughout the parameter space considered here, rendering the presence or absence of H$_2$ irrelevant as far as the thermal evolution of the gas is concerned. Second, the ratio of the ISRF strength to the gas density must also be low, typically $G_0/n \sim 0.01$, or else not enough H$_2$ will survive to provide effective cooling.

In the extreme case where $G_0 = 0$, i.e. when there is no interstellar radiation field present, we predict that H$_2$ will dominate over a wide range of physical conditions, in good agreement with the results of the previous study of Jappsen et al. (2007). On the other hand, when the radiation field is strong, our results show that H$_2$ cooling will be ineffective unless the gas density is already large. In a highly turbulent system (e.g. Walch et al. 2011) or in one which is undergoing large-scale gravitational collapse, such as a high-redshift protogalaxy (e.g. Bromm et al. 2001; Smith et al. 2005).
Figure 6. As Figure 2, but for a set of simulations that include the effects of H$_2$ self-shielding, with $L_{ss} = 10$ pc.
it is possible that the required densities could be achieved without the need for efficient cooling at $T < 10^4 \text{K}$, but in more quiescent systems, it is likely that the required value of $G_0/n$ can be achieved only when $G_0$ itself is small, i.e. when the interstellar radiation field is weak.

Our results therefore suggest that although H$_2$ cooling may enable star formation to occur in low metallicity systems that otherwise would be unable to cool, the effect will be strongly self-limiting: if too many stars form, the interstellar radiation field will become too strong, inhibiting further cooling and star formation.

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