Suppression of HD–cooling in protogalactic gas clouds by Lyman-Werner radiation

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ABSTRACT

It has been shown that HD molecules can form efficiently in metal–free gas collapsing into massive protogalactic halos at high redshift. The resulting radiative cooling by HD can lower the gas temperature to that of the cosmic microwave background, \( T_{\text{CMB}} = 2.7(1 + z) \text{K} \), significantly below the temperature of a few \( \times 100 \text{K} \) achievable via \( \text{H}_2 \)–cooling alone, and thus reduce the masses of the first generation of stars. Here we consider the suppression of HD–cooling by UV irradiation in the Lyman–Werner (LW) bands. We include photo–dissociation of both \( \text{H}_2 \) and HD, and explicitly compute the self–shielding and shielding of both molecules by neutral hydrogen, HI, as well as the shielding of HD by \( \text{H}_2 \). We use a simplified dynamical collapse model, and follow the chemical and thermal evolution of the gas, in the presence of a UV background. We find that a LW flux of \( J_{\text{crit,HD}} \approx 10^{-22} \text{erg cm}^{-2} \text{s}^{-1} \text{Hz}^{-1} \) is able to suppress HD cooling and thus prevent collapsing primordial gas from reaching temperatures below \( \sim 100 \text{K} \). The main reason for the lack of HD cooling for \( J > J_{\text{crit,HD}} \) is the partial photo-dissociation of \( \text{H}_2 \), which prevents the gas from reaching sufficiently low temperatures \( (T < 150 \text{K}) \) for HD to become the dominant coolant; direct HD photo–dissociation is unimportant except for a narrow range of fluxes and column densities. Since the prevention of HD–cooling requires only partial \( \text{H}_2 \) photo–dissociation, the critical flux \( J_{\text{crit,HD}} \) is modest, and is below the UV background required to reionize the universe at \( z \sim 10 – 20 \). We conclude that HD–cooling can reduce the masses of typical stars only in rare halos forming well before the epoch of reionization.

Key words: cosmology: theory – early universe – galaxies: formation – molecular processes

1 INTRODUCTION

The first generation of stars are believed to be much more massive \((\sim 100 \text{M}_\odot)\) than typical stars in stellar populations in the low–redshift universe \((\sim 1 \text{M}_\odot); \text{Bromm et al. 2002, Abel et al. 2002}\). This has many important consequences in the early universe, for reionization, metal–enrichment, the formation of seed black holes at very early times, and the observability of first-generation galaxies.

The high masses result from the thermodynamical properties of \( \text{H}_2 \), the main coolant in low–temperature gas with a primordial composition. In particular, \( \text{H}_2 \)–cooling becomes ineffective at temperatures below \( \sim 200 \text{K} \). HD molecules, can, in principle, cool the gas to much lower temperatures, but until recently, the abundance of HD in the early universe was believed to be too low for it to be important.

It has recently been pointed out that significant HD can form in metal–free gas, due to non-equilibrium chemistry, provided that the gas has a large initial electron fraction. This can occur, for example, in “fossil” gas that was ionized by a short-lived massive star, prior to it being extinguished, or in collisionally-ionized gas with virial temperatures above \( \approx 10^4 \text{K} \). It has been shown that the resulting radiative cooling by HD can then lower the gas temperature to values near that of the cosmic microwave background, \( T_{\text{CMB}} = 2.7(1 + z) \text{K} \), i.e. to \( \sim 30 \text{K} \) at \( z \sim 10 \). This would decrease the expected masses of the stars that form in ionized halos by a factor of \( \sim 10 \) below that which is possible if HD-cooling is neglected (e.g. \text{Johnson & Bromm 2003}). \footnote{Using three–dimensional simulations, \text{McGreer & Bryan 2008} found that HD lowers the expected Pop. III masses less dramatically, but still has an important effect.} Thus, a second mode of star formation has been proposed, giving rise to Pop. III.2 stars \footnote{Adopting the terminology suggested by \text{Bromm et al. 2009}.} that can form...
as soon as a small number of Pop. III.1 stars have initiated the epoch of reionization, and whose masses are only a few tens of solar masses (Nakamura & Umemura 2002; Machida et al. 2003; Nagakura & Omukai 2004; Johnson & Bromm 2006; Ripamonti 2007; Yoshida et al. 2007; Yoshida et al. 2009).

These conclusions could potentially be revised, however, due to the suppression of HD–cooling by UV irradiation of the gas cloud. Although this possibility has been raised in the literature (e.g. Johnson & Bromm 2006; Yoshida et al. 2009), previous work has not included a detailed treatment of the impact of UV irradiation on HD–cooling, including photo-dissociation of HD by radiation in its Lyman and Werner (hereafter LW) bands, taking into account the shielding that occurs in the optically thick regimes. Such UV radiation will exist in the early universe, and can suppress H2–cooling in low-mass halos at high redshifts (e.g., Haiman et al. 1997). The main goal of this paper is to assess whether HD–cooling can be similarly suppressed by UV radiation, and to compute the critical UV flux for the HD-destruction.

In order to do this, we perform “one zone” calculations with a simplified density evolution, while following the shielding that occurs in the optically thick regimes. Such UV radiation will exist in the early universe, and can suppress H2–cooling in low-mass halos at high redshifts (e.g., Haiman et al. 1997). The main goal of this paper is to assess whether HD–cooling can be similarly suppressed by UV radiation, and to compute the critical UV flux for the HD-destruction.

In order to do this, we perform “one zone” calculations with a simplified density evolution, while following the gas-phase chemistry and thermal evolution of the gas, including the impact of H2– and HD–dissociating UV radiation. In general, collapsing gas clouds become optically thick to this radiation, so that the effects of self-shielding are non-negligible. Our treatment includes self-shielding of HD and H2 shielding of both species by neutral hydrogen (HI), and shielding of HD by H2. We provide useful fitting formulae for these shielding factors, analogous to the case of H2 self-shielding studied by Draine & Bertoldi (1996) (hereafter DB96).

The rest of this paper is organized as follows. In §2 we describe our chemical, thermal, and dynamical modeling, §3 presents our results on the critical flux required to suppress HD–cooling, followed by a brief discussion of the potential cosmological implications and primary uncertainties in §4. We summarize our main results and offer our conclusions in §5. Throughout this paper, we adopt the standard ΛCDM cosmological background model, with the following parameters: ΩDM = 0.233, Ωb = 0.0462, ΩΛ = 0.721, and h = 0.701 (Komatsu et al. 2009).

2 MODEL DESCRIPTION

The formation of HD occurs primarily through the following reaction sequence (e.g., Galli & Palla 2002):

\[ \text{H} + e^- \rightarrow \text{H}^+ + h\nu \]  (1)

\[ \text{H} + \text{H}^+ \rightarrow \text{H}_2 + e^- \]  (2)

\[ \text{D}^+ + \text{H}_2 \rightarrow \text{HD} + \text{H}^+. \]  (3)

Thus, in order to form a significant abundance of HD, a large initial electron fraction is required to catalyze the formation of H2 (see, e.g., Johnson & Bromm 2006, and references therein). In primordial gas this can be achieved by photoionization (e.g. by short-lived Pop III.1 stars), or by collisional ionization (in sufficiently massive halos). We model the first case by a constant, low-density gas, initially at a density comparable that of the intergalactic medium (IGM) at high redshift, \( n \approx 10^{-7} (1 + z)^3 \text{ cm}^{-3} \), and temperature \( T \approx 10^4 \text{ K} \).

We model the second case by a pre-imposed density evolution obtained from the spherical collapse model.

2.1 One-Zone Spherical Collapse Model

We adopt the model for homologous spherical collapse that has been used in several previous studies (e.g. Omukai et al. 2008, hereafter OSH08). This simple one-zone treatment prescribes the density evolution of the baryonic and dark matter (DM) components of a collapsing halo. Both are initialized with zero velocity at the turnaround redshift, set throughout this paper to \( z = 17 \). The density of the infalling gas evolves on the free-fall timescale and that of the DM is given by a top-hat overdensity until virialization, after which it remains constant at its virial value. Compressional heating is included in the thermal model, along with the processes listed in §2.2.

Unless stated otherwise, we take the radius of the cloud to be \( R_c = \lambda_J / 2 \), where the Jeans length is given by

\[ \lambda_J = \sqrt{\frac{\pi k_B T_{\text{gas}}}{G \rho_{\text{gas}} m_p}}, \]  (4)

Here \( k_B \) is Boltzmann’s constant, \( T_{\text{gas}} \) is the gas temperature, \( \mu \) is the mean molecular weight, and \( m_p \) is the mass of the proton. Note that the size of the cloud is required, in practice, only in our calculations of the self-shielding factors (see below), in order to specify the column densities of H2, HD, and HI.

While this model is a vast simplification of the physics of a collapsing halo, it nonetheless has been shown to mimic the thermal and chemical evolution seen in full three-dimensional hydrodynamical simulations very well (see, e.g., Shang et al. 2010 – hereafter SBH10 – for a direct comparison). The exception is the shock-heating that occurs in the early stages of collapse and is not present in the one-zone model, which prescribes a smooth “free-fall” evolution. For a detailed description of the spherical collapse model, the reader is referred to the recent work by OSH08 and references therein.

2.2 Chemical and Thermal Model

We model a gas of primordial composition using a reaction network which comprises 47 gas-phase reactions amongst the following 14 chemical species (and photons): H, H+, H–, He, He+, He2+, H2, H2+, D, D+, D–, HD, HD+, and electrons. Our choices for the selection of species and their initial abundances are conventional (see, e.g., Galli & Palla 1998), but we do not include any lithium species or other potential coolants (e.g. H1+), as they contribute very little to the total cooling (e.g. Glover & Savin 2004) and are not important in the context of this paper.

2.2.1 Hydrogen and Helium Chemistry

The collisional rate coefficients for reactions among hydrogen and helium species only, and cross-sections for photoionization, are taken from the recent compilation by SBH10.
However, the rate for H$_2$ photo-dissociation ($k_{2\text{diss}}$ in the aforementioned compilation) is modified to $k_{\text{diss},H_2} = 1.39 \times 10^{-12} \times \beta \times f_{\text{shield}}$ in order to match the optically thin rate we calculate (see §2.3). The total shielding is parameterized by a shield factor, $f_{\text{shield}}$ (see below), and the rate is normalized by the parameter $\beta$, as described by in Appendix A of OM01, which specifies the intensity of blackbody radiation at the average LW band energy (12.4 eV) relative to that at the Lyman limit (13.6 eV). For the two spectral types we consider (described in §3), $\beta = 3$ for the T4-type and $\beta = 0.9$ for the T5-type.

### 2.2.2 Deuterium Chemistry

The chemical network includes 19 reactions involving the five deuterium species, for which we use the collisional rate coefficients from the compilation by Nakamura & Umemura (2002). However, we replace the rates D$_2$, D$_3$, D$_7$, and D$_9$ given therein (as referenced in the source) with the corresponding updated rates from Savin (2002) (for the charge exchange reactions, D$_2$ and D$_3$) and Galli & Palla (2002) (for D$_7$ and D$_9$). The HD photo-dissociation rate is given in §2.3 and is normalized with the $\beta$ parameter in the same manner as described above for the H$_2$ photo-dissociation rate.

We take the cosmological D/H ratio to be 4×10$^{-5}$ by number, following recent studies on HD-cooling (e.g. Johnson & Bromm 2006, Yoshida et al. 2007) and inspired by the model of Galli & Palla (1998), which provides a value of D/H = 4.3 × 10$^{-5}$. This adopted value is likely overgenerous for the primordial deuterium abundance, however, in light of recent observations, which place estimates of D/H at 2.73$^{+0.38}_{-0.75}$×10$^{-4}$ (Kirkman et al. 2004) and 2.82$^{+0.44}_{-0.44}$×10$^{-4}$ (O'Meara et al. 2006). However, decreasing the initial deuterium abundance in our models leads to less robust HD-cooling, and so only serves to strengthen our central conclusion that metal-free gas is unlikely to be cooled, by HD, to temperatures close to $T_{\text{CMB}}$.

In §4 we discuss recently updated rate coefficients for some of the most important reactions, and how their implementation affects our results.

### 2.2.3 Thermal Model

The following processes are included in the net cooling rate: collisional excitation and ionization (of H, He, and He$^+$), recombination (to H, He, and He$^+$), dielectronic recombination (to He), Bremsstrahlung, Compton cooling, and molecular cooling by H$_2$ and HD. In practice, the last two processes, as well as collisional excitation of HI, dominate in our calculations. We adopt the expression provided by Galli & Palla (1998) for H$_2$ cooling. In the fossil gas case, the HD-cooling rate is calculated using the analytic fit for low densities ($n \lesssim 10^5$ cm$^{-3}$) given by equation (5) in Lipovka et al. (2003). In the spherical collapse runs, we adopt the lengthier polynomial fit (equation 4 in the same source), which is accurate for gas densities $n \lesssim 10^8$ cm$^{-3}$.

We note that $T_{\text{CMB}}$ is a “temperature floor,” below which gas cannot cool radiatively; if the gas temperature were below $T_{\text{CMB}}$, interaction with photons in the roto-vibrational bands would heat, rather than cool the gas. In order to mimic this behavior, we multiply $\Lambda_{\text{H}_2}$ and $\Lambda_{\text{HD}}$ by a correction factor $(T - T_{\text{CMB}})/(T + T_{\text{CMB}})$. This ensures that cooling is shut-off as the temperature approaches $T_{\text{CMB}}$ from above (whereas the correction becomes negligible when $T \gg T_{\text{CMB}}$; see O转换为现代科学的表达式). Our thermal model includes heating from photo-detachment of H$^+$, high energy electrons resulting from photo-ionization of helium (see, e.g., Appendix B in Haiman et al. 1996), as well as compressional heating in the model of adiabatic collapse (see OSH08 and references therein for more details). In practice, the latter dominates in the regime of our calculations.

In order to follow the coupled chemical and thermal evolution of the gas we use the Livermore solver LSODAR to solve the stiff equations.

### 2.3 HD and H$_2$ Photo-dissociation in the Optically Thin Limit

HD and H$_2$ can be dissociated by photons with energies in the range 11.2-13.6 eV, to which the universe is largely transparent even before the IGM is reionized. Although both HD and H$_2$ have LW lines above 13.6 eV, we do not include photons above this energy, because they will have been absorbed by neutral hydrogen elsewhere in the IGM prior to reionization. Here we describe the details of the calculation for HD photo-dissociation; however, the calculation for H$_2$ is entirely analogous, so the following applies equally well to both molecules.

Excitation of the HD molecule to its $B^1\Sigma_u^+$ and $C^1\Pi_u$ electronic states and subsequent radiative decay leads to dissociation when the system decays to the vibrational continuum of the ground state, rather than back to a bound state. Here we discuss the optically thin case, in which the processing of the LW spectrum by HD itself (as well as by H$_2$ and HI) is assumed to be negligible. The dissociation rate for molecules initially in the electronic ground state with vibrational and rotational quantum numbers $(v, J)$ is given by:

$$k_{\text{diss},v,J} = \sum_{v',J'} \zeta_{v,J',v',J'} f_{\text{diss},v',J'}$$  \hspace{1cm} (5)

where $f_{\text{diss},v',J'}$ is the dissociation probability from the excited state $(v', J')$ and the pumping rate is given by:

$$\zeta_{v,J,v',J'} = \int_{\nu_{\text{th}}}^{\infty} 4\pi\sigma_{\nu} J_{\nu} h_{\nu} d\nu.$$  \hspace{1cm} (6)

Here $\sigma_{\nu}$ is the frequency-dependent cross-section of a given transition, $h_{\nu}$ is Planck’s constant, and the specific intensity just below 13.6 eV is hereafter normalized as $J_{\nu} = J_{21} \times 10^{-22}$ erg cm$^{-2}$ sr$^{-1}$ s$^{-1}$ Hz$^{-1}$. As mentioned above, in our model there is a sharp cut off in the radiation spectrum above 13.6 eV; the lower limit, $\nu_{\text{th}}$, is the frequency threshold, corresponding to the longest-wavelength photons included, $\lambda \sim 1105$ Å.

In principle, the total dissociation rate also depends on the level populations of the molecule, which in turn depend on the incident radiation field as well as the temperature and...
density of the gas; thus, the total dissociation rate should be:

\[
k_{\text{diss, tot}} = \sum_{v,J} k_{\text{diss,v,J}} f_{v,J},
\]

where \( f_{v,J} \) is the fraction of molecules initially in the ro-vibrational state denoted by \( v, J \). For simplicity, we assume that all HD and \( \text{H}_2 \) molecules are initially in the ground state (i.e., \( f_{v=0,J=0} = 1 \)). This is a reasonable approximation for low gas densities, at which the populations of higher ro-vibrational states are very small. However, the level populations of \( \text{H}_2 \) and HD reach their values at local thermodynamic equilibrium when gas densities rise to \( n \gtrsim 10^6 \text{ cm}^{-3} \), and \( n \gtrsim 10^9 \text{ cm}^{-3} \) respectively. In §[4] we discuss the differences in the dissociation rates if both molecules are assumed to be in LTE, and how this impacts the results discussed below.

We include 28 discreet spectral lines of HD and 25 of \( \text{H}_2 \), all involving transitions from from the ground electronic state \( X^1 \Sigma^+ \sum_v^p \to \text{B}^1 \Sigma^+ \sum_v^p \) and \( C^1 \Pi^+ \sum_v^p \) excited states. We use the necessary data for the Lyman and Werner bands of HD provided by Abgrall & Roueff (2006). For those of \( \text{H}_2 \), the relevant data were taken from Abgrall et al. (1993a), and Abgrall et al. (1993b). We use the updated dissociation fractions for \( \text{H}_2 \) in Abgrall et al. (2000). The numerical wavelength resolution in the calculations \( (\Delta \lambda = 5.8 \times 10^{-5} \text{ Å} \) at the lowest temperatures) is sufficient to resolve the Voigt profile of each line and explicitly account for overlap of the Lorentz wings. We find the following photo-dissociation rates in the optically thin limit: \( k_{\text{diss,HD}} = 1.55 \times 10^9 J_0 \text{ s}^{-1} \), and \( k_{\text{diss,H}_2} = 1.39 \times 10^9 J_0 \text{ s}^{-1} \) in excellent agreement with those found previously by Glover & Jappsen (2007): \( k_{\text{diss,HD}} = 1.5 \times 10^9 J_0 \text{ s}^{-1} \), and \( k_{\text{diss,H}_2} = 1.38 \times 10^9 J_0 \text{ s}^{-1} \). Here \( J_0 \) denotes the intensity at the average LW band of HD and \( \text{H}_2 \), with energy 12.4 eV, as discussed above.

### 2.4 Self-Shielding of HD and \( \text{H}_2 \)

When sufficiently high column densities of HD or \( \text{H}_2 \) build up, \((N_{\text{HD}}, N_{\text{H}_2} \gtrsim 10^{13} \text{ cm}^{-2})\), the LW bands become optically thick and the rates of photo-dissociation are suppressed. We parameterize this effect by a shield factor, \( f_{\text{shield}} \), akin to that given by DB96 in their study of \( \text{H}_2 \) self-shielding. In particular, \( f_{\text{shield,HD}}(N_{\text{HD}}) = k_{\text{diss,HD}}(N_{\text{HD}})/k_{\text{diss,HD}}(N_{\text{HD}} = 0) \) where \( k_{\text{diss,HD}}(N_{\text{HD}} = 0) \) is the dissociation rate in the optically thin limit (equation [2]), and the shield factor for \( \text{H}_2 \), \( f_{\text{shield,H}_2} \), is analogously defined. Our treatment of \( \text{H}_2 \) self-shielding differs from the previous study by DB96 in that we assume all \( \text{H}_2 \) is in the ro-vibrational ground state (as described above), while the latter used a model allowing for populations in higher ro-vibrational levels due to collisional excitation and “UV pumping” by the incident radiation field. Nonetheless, we find that a good analytical fit for both \( \text{H}_2 \) and HD self-shielding is provided by the same functional form as equation (37) for \( f_{\text{shield,HD}} \). We also find that the self-shielding behavior of the two molecules is nearly identical, (see Figure 1), which might be expected on the basis of the similarity in their electronic structures.

Thus, we use the following fit for both \( f_{\text{shield,HD}}(N_{\text{HD}}) \) and \( f_{\text{shield,H}_2}(N_{\text{HD}}, T) \):

\[
f_{\text{shield}}(N, T) = \frac{0.9379}{(1 + x/D_\text{D})^{1.879}} + \frac{0.03465}{(1 + x)^{0.475}} \times \exp[-2.293 \times 10^{-4}(1 + x)^{0.5}],
\]

where \( x = N/8.465 \times 10^{13} \text{ cm}^{-2} \), \( N \) is the column density of the self-shielding species, \( D_\text{D} \equiv b_\text{D}/10^5 \text{ cm} s^{-1} \), and the Doppler broadening parameter, \( b_\text{D} \), depends on the mass of the molecule (which accounts for the slight difference in the self-shielding formula for the two molecules), as well as the temperature.

### 2.5 Shielding by HI and Mutual Shielding of \( \text{H}_2 \) and HD

In addition to self-shielding, HD and \( \text{H}_2 \) can also shield each another, and both can be shielded by HI, which has absorption lines in the range 11.2-13.6 eV; thus, suppression of the photo-dissociation rates depend on the relative strengths and positions of the HD, \( \text{H}_2 \), and HI lines, as well as the column densities of each species, \( N_{\text{HD}}, N_{\text{H}_2}, \) and \( N_{\text{HI}} \).

[4] The similarities in the line strengths of \( \text{H}_2 \) and HD, quantified by the product of the oscillator strength and dissociation fraction, can be seen in Figure 2 below.
We include the first nine Lyman HI lines in the relevant wavelength range; while the line center of the Lyα line is outside this range, we nevertheless include it, as its contribution to the shielding becomes important due to line broadening at high HI column densities. For illustration, in Figure 2 we show the positions and strengths of the most significant lines of each species.

2.5.1 Shielding of HD by H₂ and HI

Taking shielding into account, the contribution to the HD–dissociation rate for a particular line at frequency ν becomes:

\[ k_{\text{diss,HD},\nu}(N_{\text{HD}}) = k_{\text{diss,HD},\nu}(N_{\text{HD}} = 0) \exp(-\tau_\nu), \]

where the optical depth is given by

\[ \tau_\nu = \sigma_{\text{HD},\nu} N_{\text{HD}} + \sigma_{\text{HI},\nu} N_{\text{HI}} + \sigma_{\text{H}_2,\nu} N_{\text{H}_2}. \]

While HD self-shielding becomes important for \( N_{\text{HD}} \gtrsim 10^{13} \text{ cm}^{-2} \), the offsets in the wavelength of the neighboring absorption lines (typically of order \( \sim \lambda \)) prevent H₂ and HI from effectively shielding HD until their column densities are very high, \( N_{\text{H}_2} \gtrsim 10^{20} \text{ cm}^{-2} \), and \( N_{\text{HI}} \gtrsim 10^{23} \text{ cm}^{-2} \). At these critical densities, which are essentially independent of \( N_{\text{HD}} \), the HD lines start to significantly overlap and the optical depth due to H₂–shielding is \( \sim \) a few at all wavelengths. In Figure 3 we show the evolution of all three column densities, as a function of the particle number density, in our one-zone collapse runs with \( J = 0 \) for halos with virial temperatures both above and below \( 10^4 K \) (see below). This figure shows that all three column densities reach the values where shielding becomes efficient, and thus a full calculation of the combined self-shielding is warranted.

We provide a fitting formula to model the total shielding of HD, \( f_{\text{shield,HD}}(N_{\text{HD}}, N_{\text{H}_2}, N_{\text{HI}}, T) \), representing the total combined shielding factor of HD, including shielding by H₂ and HI (equations 11 and 12 below), which is accurate to within a factor of two over a wide range of column densities, i.e. up to \( N_{\text{HD}} \approx 10^{20} \text{ cm}^{-2} \), \( N_{\text{H}_2} \approx 10^{22} \text{ cm}^{-2} \), \( N_{\text{HI}} \approx 10^{24} \text{ cm}^{-2} \), and gas temperatures up to \( \approx 10^3 K \) (HD–cooling is unimportant at temperatures above this value in any case):

\[ f_{\text{shield,HD}} = f_{\text{shield}}(N_{\text{HD}}, T) \times f_1(N_{\text{HI}}) \times f_2(N_{\text{H}_2}) \]

\[ f_i = \frac{1}{(1 + x_i)^{\gamma_i}} \exp(-\beta_i x_i). \]

Here \( x_i \equiv N_i/\gamma_i \) and the index \( i \) takes the value \( i = 1 \) or 2 to denote the relevant quantity for HI or H₂ respectively. The coefficients \( \alpha, \beta, \) and \( \gamma \) are given in Table 1.

This fit is described by a product of three separate functions, \( f_{\text{shield,HD}}(N_{\text{HD}}, T), f_{\text{shield,H}_2}(N_{\text{H}_2}), \) and

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
Species & \( \alpha \) & \( \beta \) & \( \gamma \) (cm\(^{-2}\)) \\
\hline
1. HI & 1.620 & 0.149 & \( 2.848 \times 10^{23} \) \\
2. H₂ & 0.238 & 0.00520 & \( 2.339 \times 10^{19} \) \\
\hline
\end{tabular}
\caption{Coefficients for the fitting formula for \( f_{\text{shield,HD}}(N_{\text{HD}}, N_{\text{H}_2}, N_{\text{HI}}, T) \), representing the total combined shielding factor of HD, including shielding by H₂ and HI (equations 11 and 12). The analytic fit for self-shielding is given in equation 8.}
\end{table}
$f_{\text{shield,HI}}(N_{HI})$, which represent the shielding of HD due to each of the three species alone (eq. [11] above). Note that since the H$_2$ and HI lines shield HD by their Lorentz wings, rather than their thermal cores, these factors (unlike HD self-shielding) do not depend on temperature.

In general, one does not expect that the combined shielding factor is separable into a simple product of the three individual shielding factors. The full expression for $f_{\text{shield,HD}}(N_{H_2}, N_{HI}, N_{HI}, T)$ is a sum over all of the individual cross-sections of the HD lines, each suppressed by the frequency-dependent total optical depth (eq. [10]), divided by the optically thin rate. However, we have found that in practice, when suppression by nearby HI lines is negligible ($N_{HI} \lesssim 10^{23}$ cm$^{-2}$), one HD line is much stronger than all others (at $\approx 950\,\AA$, see Figure 2). Since this single line dominates the dissociation rate, the shield factor reduces to the simple product (eq. [11] above). In the regime of relatively strong HI shielding ($N_{HI} \approx 10^{24}$ cm$^{-2}$), a few HD Lyman lines together dominate the dissociation rate. However, we find that the product $\sigma_\lambda \times f_{\text{diss,}\lambda}$ for these lines (at $\sim 960$, $\sim 980$, and $\sim 990\,\AA$) are similar. If we approximate that these lines have identical strengths, the total shielding factor again reduces to the simple product in equation [11] above. Because these line strengths are not precisely equal, the largest discrepancies in the product formula and ‘true’ shielding behavior are seen at $N_{HI} = 10^{24}$ cm$^{-2}$. However, in general, we find that this simple product is accurate, to within a factor of $\sim$two, at the low temperatures ($T \lesssim 200$ K) and the high column densities of interest.

Figure 4 shows the results of the exact shielding factor calculations for a gas temperature of $T = 200$ K, and compares these to the analytical fits for a number of combinations of the three column densities. The largest deviations are seen in the bottom panel, for $N_{HI} = 10^{24}$ cm$^{-2}$, and at H$_2$ and HD column densities of $N_{H_2} = 10^{22}$ cm$^{-2}$ and $10^{24}$ cm$^{-2} \lesssim N_{HD} \lesssim 10^{25.5}$ cm$^{-2}$. In this regime, the accuracy of the fitting formulae is somewhat worse than a factor of two. However, in practice, this column density combination – with relatively low $N_{HD}$ and exceedingly high values of both $N_{H_2}$ and $N_{HI}$ – does not occur in our calculations (see Figure 3).

### 2.5.2 Shielding of H$_2$ by HI and HD

The shielding of H$_2$ by HD and HI is entirely analogous to that discussed in the preceding section, so we will limit the discussion here to a few noteworthy points. Most importantly, we find that HI shielding of H$_2$ is nearly identical to HI shielding of HD; accordingly, we model both with the fitting formula for $f_{\text{shield,HI}}(N_{HI})$, given by equation [12] and Table 1. The explanation for this is similar to that given above; namely, the relative positions of the H$_2$ and HI lines is such that only the wings of the HI lines shield H$_2$ when the column densities of $N_{HI}$ are sufficiently large ($N_{HI} \gtrsim 10^{23}$). Because the H$_2$ and HD lines are comparably spaced relative to the HI lines, the shielding effect of HI should indeed be similar for both.

When the HI column is below the critical level for strong shielding of H$_2$, we find that a few Lyman lines together dominate the dissociation rate, and that the product $\sigma_\lambda \times f_{\text{diss,}\lambda}$ for these lines (at $\sim 945$, $\sim 980$, and $\sim 990\,\AA$) are

Figure 4. The combined HD shielding factor, including self-shielding and shielding by H$_2$ and HI. Several combinations of column densities are shown, as labeled, near the critical column densities for HI and H$_2$ shielding. The solid curves show the exact numerical calculations, and the dotted curves show the values obtained from a fitting formula (equations 8, 11, and 12 and Table 1).
similar. At larger neutral hydrogen columns (\(N_{\text{HI}} \approx 10^{23}\)), a single Lyman H\(_2\) line makes the dominant contribution – by a large margin over all others – to the dissociation rate. Thus, the total shielding factor can again be simply modeled by a product of the shielding formulae, given in equations 8, 12 and Table 1:

\[
\mathcal{f}_{\text{shield}, \text{H}_2} = \mathcal{f}_{\text{shield}, \text{H}_2} (N_{\text{HI}}, T) \times f_1 (N_{\text{HI}})
\]

The results of the exact shielding factor and comparison to this analytical fit are shown in Figure 5 for a gas temperature of \(T = 200\, \text{K}\).

In principle, HD can also shield H\(_2\), but in practice this effect will likely always be negligible, as the HD column density is typically dwarfed by those of \(\text{H}_2\) and HI. Thus, our treatment does not include HD shielding of H\(_2\).

### 3 RESULTS

To assess whether HD-cooling can be one-suppressed by a persistent LW background, we ran our one-zone models at various different specific intensities \(J_{21}\). Unless stated otherwise, the spectrum of the radiation is modeled as a black-body with a temperature of \(10^5\, \text{K}\), approximating the hard spectrum expected to characterize Pop III.1 stars (Tumlinson & Shull 2000; Bromm et al. 2001; Schaerer 2002). For comparison, in § 3.2 below, we investigate the effects of illumination by a cooler blackbody, \(T \sim 10^4\, \text{K}\), intended to represent the softer spectrum of a more typical metal-enriched stellar population. These are referred to hereafter as types ‘T5’ and ‘T4’ respectively (SBH10).

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\(^5\) The fractional abundance of HD relative to that of \(\text{H}_2\) could exceed the cosmological D/H ratio by a large factor, owing to chemical fractionation at low temperatures (see, e.g., Galli & Palla 1998). However, it never exceeds \(~ 10^{-2}\) in our models.

We use a Newton-Raphson scheme to determine the strength of the LW radiation required to keep the gas temperature greater than a factor of \(~ 2\) above that reached in the absence of any LW radiation, \(T_{\text{min}}, J_{21} = 0\), on the timescales described below; this is referred to hereafter as the critical intensity: \(J_{\text{crit}, \text{HD}}\) (in the usual units of \(10^{-21}\, \text{erg cm}^{-2}\, \text{sr}^{-1}\, \text{s}^{-1}\, \text{Hz}^{-1}\)).

### 3.1 HD-Cooling in Constant-Density Fossil HII Gas

The first of the physical scenarios we consider is a “fossil” HII region, which could occur in a patch of the low-density IGM that has been photo-ionized and heated by a short-lived massive star (see, e.g., Oh & Haiman 2003), or possibly in a denser shell of primordial gas, compressed by shocks from a supernova (SN).

We are interested in whether gas with such fossil ionization can cool efficiently in the presence of a LW background and return, via HD cooling, to a state close to its initial low-entropy state, prior to the ignition of the ionizing source (or prior to its shock heating).

In a first set of runs, we assume that the number density remains constant at the low value of \(n = 10^{-2}\, \text{cm}^{-3}\), characteristic of a slightly over-dense (by \(~ 1\) factor of 10) region of the IGM at \(z = 10\). We find that in such a rarefied patch, the gas is not able to cool on a realistic timescale, because the HD–cooling time is longer than the present age of the universe even in the absence of any LW background. The thermal evolution of the gas in this case is shown by the right set of (purple) curves in the upper panel of Figure 6.

The corresponding fractional abundances of electrons, H\(_2\), and HD are shown in the lower panel of the same figure. The figure extends to a total elapsed time that exceeds the Hubble time, and shows that there is, technically, a critical flux \((J_{\text{crit}, \text{HD}} \approx 10^{-6})\) that would suppress the HD–cooling that would otherwise occur after a few \(10^{10}\) seconds. This, of course, is unphysical, and in practice, the question of HD–cooling being suppressed by UV radiation is moot for such low-density gas. Nevertheless, the figure illustrates the chemical/thermal behavior, and also provides a useful check on our code (see below).

In the second set of runs, the total particle number density was set to a higher value of \(n = 10^2\, \text{cm}^{-3}\). This is an unphysically high density for a characteristic “flash–ionized” fossil region in the low-density IGM, but may represent primordial gas compressed by SN shocks. In the no-flux case, we reproduce the main result of Johnson & Bromm (2004), namely that HD-cooling allows the gas to reach the temperature of the CMB in a time that is shorter than the Hubble time. This gas, however, is optically thin to radiation in the LW bands, and dissociation of HD (as well as of \(\text{H}_2\)) is efficient. We find that for \(J_{21} \gtrsim 10^{-2}\), the gas cannot cool to temperatures less than \(~ 200\, \text{K}\). This is shown in the top panel of Figure 5 by the left set of (blue) curves.

The above two cases \((n = 10^{-2}\, \text{cm}^{-3}\) and \(n = 10^2\, \text{cm}^{-3}\) serve to illustrate an important point (and a check on our code). All of the relevant timescales for the system, including the formation timescale for HD \((t_{\text{form}})\), the HD cooling time \((t_{\text{cool}})\), and the (HI+e \rightarrow HII) recombination time \((t_{\text{rec}})\), scale as \(1/n\). The exception is the photo–dissociation timescale, which scales with the flux strength, \(t_{\text{diss}} \propto J_{21}^{-1}\).
Figure 6. The top panel shows the thermal evolution of constant density gas that is initially fully ionized. The right/left set of solid purple/blue curves adopt densities of $10^{-2}$ and $10^{-3}$ cm$^{-3}$, appropriate for a flash-ionized patch of the IGM and for primordial gas compressed by a SN–shock, respectively. In both cases, we show the evolution when the gas is exposed to LW backgrounds of various intensities, as labeled. The dashed lines show the temperature reached in deuterium-free gas, in the absence of any LW. The temperature of the CMB, $T_{\text{CMB}} = 2.7(1+z)$, is shown by the dotted blue curve (starting from $z = 20$). The bottom panel shows the fractional abundances of electrons (light blue dotted lines), HD, and H$_2$ (solid blue and green lines respectively) in the low–density case. The fractional abundances are not shown in the case of the shock-compressed gas for the sake of clarity, and because the patterns they follow are identical to those shown in the lower panel. This figures shows that there is a critical flux, $J_{\text{crit,HD}} = 3.8 \times 10^{-2} (n/10^{2} \text{ cm}^{-3})$, that suppresses HD–cooling and prevents the gas from reaching the CMB temperature.

in the absence of shielding. Thus, the history of the system should only depend on $J_{21}/n$ when the gas is rescaled accordingly.$^6$ This simple scaling is evident by the two sets of (purple and blue) curves in the top panel of Figure 6. Most importantly, there is indeed a critical flux that prevents the gas from reaching the CMB temperature by HD cooling; in constant density gas with a high initial electron fraction, we find the value of this flux is $J_{\text{crit,HD}} = 3.8 \times 10^{-3} (n/10^{2} \text{ cm}^{-3})$.

Finally, an interesting question is whether HD–cooling prevented, for the cases in which $J_{21}$ exceeds the critical value, by direct photo–dissociation of HD, or the inability of sufficient HD to form due to H$_2$ photo–dissociation. To answer this question, we performed runs in which the H$_2$–dissociation was artificially turned off. In these runs, we find that the gas is still able to cool to $T_{\text{CMB}}$ for $J_{21} \approx 4 \times 10^{-2}$, illustrating that the LW flux prevents HD–cooling via H$_2$ destruction, rather than via direct HD–dissociation. This point has been discussed by previous authors, e.g. Nakamura & Umemura (2002) showed that a critical abundance of H$_2$, $x_{H_2} \gtrsim 10^{-6}$ is required for the gas to reach sufficiently low temperatures for HD to become the dominant coolant ($T \lesssim 150 \text{K}$), and therefore H$_2$ dissociation can prevent HD–cooling (Yoshida et al. 2007). The minimum temperature reached by fossil ionized primordial gas in the absence of HD, and the dependence of this minimum temperature on gas density and LW flux was also discussed in detail by Oh & Haiman (2003).

3.2 HD Cooling in Collapsing Halos

3.2.1 HD Cooling in Halos with $T_{\text{vir}} > 10^4 \text{K}$

It has been shown that primordial gas in the late stages of runaway gravitational collapse can reach temperatures close to $T_{\text{CMB}}$ via HD–cooling, provided that a large initial ionization fraction exists (e.g. Johnson & Bromm 2006; see also Machida et al. 2005). This scenario can be realized in sufficiently massive halos, which are collisionally ionized upon shock-heating to their virial temperatures. The post–shock gas can cool faster than it recombines, leaving a large out–of–equilibrium electron fraction to catalyze both H$_2$ and HD formation (e.g. Shapiro & Kang 1987; Susa et al. 1998; Oh & Haiman 2004). It may also be the case that “pre-ionized” halos exist within fossil HII regions, which will undergo a phase of efficient HD–cooling upon collapse (Johnson & Bromm 2004). This scenario, however, is less plausible: a halo large enough to remain bound once photo-heated (to $T \gtrsim 10^4 \text{K}$) may be difficult to completely ionize, as the large HI column densities will lead to non-negligible HI self-shielding (Dijkstra et al. 2004); flash–ionization by a single short–lived star (required to allow subsequent recombination and cooling) is even less likely.

Regardless of the nature of the initial ionization, Figure 7 shows the thermal evolution of the collapsing gas exposed to LW backgrounds of various intensities. The initial number density is set to the characteristic baryon density in halos upon virialization,

$$n \approx 0.3 \text{ cm}^{-3} \left( \frac{1 + z_{\text{vir}}}{21} \right)^3,$$

and the gas begins cooling from the temperature $T \approx 10^4 \text{K}$ (quickly established either by a period of photo–heating, or by shock–heating to near the virial temperature, accompanied by rapid HI cooling).

Of primary importance in this case – as opposed to the fossil gas discussed in the previous section – are the large column densities of HD and H$_2$ that build up and shield both populations against the LW background. Furthermore, the collapse itself leads to more efficient formation of both molecules because the formation timescale, as mentioned above, scales as $t_{\text{form}} \propto 1/n$. Consequently, the critical intensity should be larger than that found for the low-density fossil gas. This is indeed borne out by our results; nevertheless, as the comparison between the solid and the dashed curves (the latter representing deuterium-free

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$^6$ The interested reader can find a much more detailed discussion of this point for the analogous case of H$_2$ cooling in Oh & Haiman 2002.
Figure 7. Thermal evolution of initially ionized gas, collapsing in a massive halo \( T_{\text{vir}} \gtrsim 10^4 \text{K} \) exposed to LW backgrounds in the range near the critical value, \( J_{\text{crit,HD}} = 3.6 \times 10^{-1} \) (solid curves). The incident spectrum is that of a blackbody with a temperature of \( 10^4 \text{K} \), characteristic of massive Pop III.1 stars. The turnaround redshift is set to \( z = 17 \) and the temperature is initialized \( T \approx 10^4 \text{K} \). The dashed curves show, for comparison, the temperature evolution in deuterium-free gas, exposed to the same LW fluxes. The dotted curves show the thermal evolution when HD-dissociation is artificially switched off, for the same values of \( J_{21} \), as labeled. This illustrates that, except in a small range of flux intensities, the destruction of \( \text{H}_2 \) by LW photons, rather than direct HD photo-dissociation, is the primary factor determining the minimum temperature reached in the gas. The temperature of the CMB is shown by the blue dotted curve.

Gas) in Figure 7 shows, the effect of HD–cooling is still almost entirely erased for the relatively low values of \( J \gtrsim 1 \). The critical intensity in this case, as defined above, is found to be \( J_{\text{crit}} = 3.6 \times 10^{-1} \).

This threshold value is most notable for being approximately five orders of magnitude lower than the critical flux required to completely suppress \( \text{H}_2 \)-cooling in the same halos. As shown in SBH10, the latter critical flux in halos with \( T_{\text{vir}} \gtrsim 10^4 \text{K} \) is \( J_{\text{crit},\text{H}_2} \gtrsim 10^3 \). This large critical flux corresponds to the value that results in an \( \text{H}_2 \)-photo–dissociation rate that matches the \( \text{H}_2 \) formation rate, at the critical density of \( n \sim 10^4 \text{ cm}^{-3} \) of \( \text{H}_2 \) (see the earlier work by O01 for a detailed discussion of the physics determining \( J_{\text{crit},\text{H}_2} \) in primordial gas without ionization/shock–heating). This \( J_{\text{crit},\text{H}_2} \approx 10^4 \) separates gas in which \( \text{H}_2 \)-cooling is fully suppressed (with the gas temperature remaining near \( 10^4 \text{K} \)) and halos in which \( \text{H}_2 \) cooling significantly lowers the temperature. A point that was also found (but not emphasized) by SBH10 (and also by O01) is that even for \( J_{21} \) well below \( J_{\text{crit},\text{H}_2} \), the minimum temperature to which the gas can cool via \( \text{H}_2 \) can be significantly elevated. This is also clearly visible in the deuterium-free runs in Figure 7.

The minimum temperature is \( \sim \) 150K for \( J_{21} = 0 \), but is elevated to \( \sim \) 300K already for \( J_{21} = 1 \).

The behaviour of the gas, and the reason for the elevated temperature, can be described as follows (see a detailed discussion in the constant–density case in Oh & Haiman 2002). Starting from \( T \approx 10^4 \text{K} \), the gas initially cools via \( \text{H}_2 \) and recombines on time–scales much shorter than either the photo–dissociation or the free–fall timescale. However, when the temperature is lowered to a \( J \)-dependent critical value of a few\( \times 10^4 \text{K} \), \( \text{H}_2 \)-dissociation becomes important, limiting the \( \text{H}_2 \) abundance, and reducing the cooling. The cooling time eventually becomes comparable to the free–fall time, resulting in the sharp turn away from the nearly vertical directions of the \( n - T \) curves at the initial density in Figure 8. For higher fluxes, this subsequently results in an elevated gas temperature (at fixed density). Eventually, the compressional heating rate becomes equal to the \( \text{H}_2 \)-cooling rate, setting the temperature minimum.

It is worth noting that for sub–critical values of \( J_{21} \leq J_{\text{crit,HD}} \), HD is able to cool the gas to temperatures below 150K, but the LW background still has the subtle effect of raising the minimum temperature to which the gas can cool via HD.

As in the constant density case, an interesting question is whether ultimately the HD–cooling is controlled by direct photo–dissociation of HD, or by \( \text{H}_2 \)-dissociation. To answer this question, we repeated the runs shown in Figure 7 under the same conditions, but with HD dissociation artificially switched off (the results are shown by the dotted lines in Figure 7). In this case, we find again that (except in a narrow range of LW intensities near \( J_{21} \sim 4 \times 10^{-1} \)), direct photo–dissociation of HD does not determine the minimum temperature reached in the gas. Rather, it is the diminished abundance of \( \text{H}_2 \) in the presence of the LW background that regulates the abundance and thereby the cooling efficiency of HD.

We have also investigated the thermal evolution of the gas when \( \text{H}_2 \) is artificially prevented from dissociating (not shown), but the physical set-up is otherwise analogous to the runs (in which deuterium is included) shown in Figure 7. This “academic” exercise is useful in order to determine the critical flux that would prevent HD–cooling entirely by direct HD photo–dissociation. In the analogous case for \( \text{H}_2 \), as mentioned above, \( J_{\text{crit},\text{H}_2} \) is traditionally defined as the specific intensity capable of completely suppressing \( \text{H}_2 \)-cooling, thereby preventing the gas from falling below the temperatures reached by atomic line cooling, \( T \sim 8 \times 10^3 \text{K} \) (O01, OSH08, SBH10). We find that for \( J \gtrsim 6 \times 10^3 \), the cooling history of the gas is nearly identical to that of deuterium-free gas in the absence of a LW background. Thus, the intensity required to fully suppress HD–cooling by direct HD–dissociation is comparable to that of \( \text{H}_2 \) (the latter was found by the latest studies (SBH10) to be \( \sim 1.2 \times 10^4 \), but we find a factor of \( \sim 5 \) greater critical value for \( \text{H}_2 \); see below). In fact, this is not surprising, given that the photo–dissociation timescales \( (t_{\text{diss}} = k_{\text{diss}}(N = 0) \times f_{\text{shield}})^{-1} \) are very similar for the two molecules.

3.2.2 \( T_{\text{vir}} > 10^4 \text{K} \) Halos Illuminated by ‘T4’ Radiation

Up to this point, we have considered only incident radiation with the hard spectrum expected to characterize Pop III.1.

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stars (‘T5’). In the case of a collapsing halo, it is reasonable to ask about the effects of irradiation by the more the typical stellar spectrum (‘T4’), on HD-cooling.

Figure 8 shows the temperature evolution in the gas irradiated by a T4 spectrum of various intensities. It is clear that HD is considerably more fragile in the presence of this softer spectrum, withstanding a LW flux no greater than a feeble \( J_{\text{crit, HD}} = 10^{-2} \). This is not surprising in the light of studies that have found the same effect for \( \text{H}_2 \) (O01; OSH08; SBH10), namely, that \( \text{H}_2 \)-cooling is much more effectively suppressed by the T4 type spectrum. The reason is the diminished abundance of hydride (\( \text{H}^- \)), an intermediary in the formation of both \( \text{H}_2 \) and HD. Hydride, whose ionization threshold is 0.76eV, is more efficiently photo-dissociated by the softer spectral type (O01, SBH10). This again is a manifestation of how an external radiation field can regulate HD-cooling via the destruction of an intermediate in its formation pathway.

### 3.2.3 HD Cooling in \( T_{\text{vir}} < 10^4 \)K Halos

It has long been known that pristine gas in the first minihalos cannot form sufficient \( \text{H}_2 \) to cool below a few hundred Kelvin (e.g. Haiman et al. 1996). Because free electrons act to catalyze the formation of HD, as well as \( \text{H}_2 \), it is not surprising that HD abundances remain too low in such halos to play a significant role in cooling (e.g. Johnson & Bromm 2002, and references therein). This is borne out by our results, shown in Figure 9 for a halo that begins collapsing from a temperature of \( T \approx 20\text{K} \) at the turnaround redshift, \( z = 17 \), and is illuminated by a ‘T5’ spectrum. This is the same configuration as in Figure 8 except that the initial temperature is assumed to be low (i.e., lacking any strong shocks able to collisionally excite or ionize the gas).

We include a discussion of this scenario for the purpose of highlighting a few noteworthy points. First, we find a critical flux for full \( \text{H}_2 \)-dissociation in this case (as it is traditionally defined, see § 3.2.4 above) of \( J_{\text{crit, HD}} = 6.1 \times 10^3 \), which is a factor of \( \sim 5 \) greater than that found in the recent study by SBH10. This difference owes to our use of the analytic fit for \( \text{H}_2 \) self-shielding (equation 5), which assumes all molecules are initially the ground state, while SBH10 used the shield factor fit (equation 36) from DB96, which gives a very good approximation to the self-shielding when the \( \text{H}_2 \) roto–vibrational levels reach LTE populations.

This illustrates an important point that will be discussed in greater depth in § 4, namely, self-shielding is less effective when higher ro-vibrational states of the molecule are populated (see more discussion in § 4 below). It is also worth noting that we find \( J_{\text{crit, HD}} = 6 \times 10^3 \) – a factor of 2 lower than that found by SBH10 – if the self-shielding is modeled instead with the more accurate formula provided by DB96 (equation 37), rather than the power-law fit (equation 36) used by SBH10. In general, the “real” LW intensity required to kill \( \text{H}_2 \)-cooling entirely will depend on the detailed ro-vibrational distribution of \( \text{H}_2 \) molecules. The values of \( J_{\text{crit, HD}} \) found here using the ground-state vs LTE shielding treatments serve to bracket the range for the true critical threshold, with the former approximating the upper limit on \( J_{\text{crit, HD}} \). The threshold flux in this case is of particular interest as it has important implications for the number of halos that remain \( \text{H}_2 \)-poor, and thus for the abundance of halos collapsing directly to massive seed black holes, because such halos probe the rare, exponential tail of the fluctuating UV background (Dijkstra et al. 2008). (The interested reader is encouraged to see SBH10 for a detailed discussion of these issues.)

Second, while there is a clear bifurcation in the cooling history of the gas around the \( J_{\text{crit, HD}} \) discussed above, we note that it does not cool to the low temperatures required for HD-cooling to become important (\( T \sim 150\text{K} \)) even when the intensity is well below this threshold (indeed, even in the absence of any LW background). Thus, again, \( \text{H}_2 \) abundance plays the primary role in regulating HD-cooling, though in this case the result is simpler: HD–cooling never becomes important because \( \text{H}_2 \)-cooling is never strong enough for the gas temperature to fall below \( \approx 200\text{K} \).

Finally, in this case HI shielding serves to increase the threshold LW flux by \( \sim 40\% \) above that which \( \text{H}_2 \) could otherwise withstand. By contrast, \( J_{\text{crit, HD}} \) found in the two preceding sections is not sensitive to the effect of \( \text{H}_2 \) shielding by HI, in spite of its strong dependence on the \( \text{H}_2 \) abundance. This is because, in the models of \( T_{\text{vir}} \geq 10^4 \text{K} \) halos, the HI column density does not reach the critical value above which it effectively shields \( \text{H}_2 \) (\( N_{\text{HI}} \geq 10^{23} \text{ cm}^{-2} \)) until very late in the collapse (i.e., once the particle density has reached \( n \geq 10^{5.5} \text{ cm}^{-3} \)). However, sufficiently high column densities of HI do build up earlier in the high-J\(_2\) runs of \( T_{\text{vir}} < 10^4 \text{K} \) halos, resulting in the modest increase in \( J_{\text{crit, HD}} \) as quoted above.

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gen is commonly taken to be Here the number of UV photons required to ionize hydro-
gas. There are no strong shocks able to collisionally excite or ionize the
gas.

The results for the halo illuminated by a T4 spectrum are omitted here because they do not significantly differ from those described above for the T5 case, except that H2-cooling is disabled by a much lower LW flux, as shown already by O01.

4 DISCUSSION

The most significant result found in this paper is that a UV flux can prevent HD–cooling from lowering the gas temperature to near that of the CMB. In particular the threshold value in collapsing halos, $J_{\text{crit,H2}} \sim 4 \times 10^{-1}$, is approximately five orders of magnitude lower than the critical flux required to completely suppress H2-cooling in the same halos. As explained in § 3.2.1, this large difference arises because even for $J_{21}$ well below $J_{\text{crit,H2}}$, the minimum temperature to which the gas can cool via H2 is significantly elevated, so that HD formation and cooling is not activated.

What are the cosmological implications if a LW background prevents halos from cooling via HD line emission? The critical flux we find should be compared to the level of the LW background $J_{\text{bg}}$ expected at the redshifts we consider. For reference, an estimate of the background as a function of redshift is provided by requiring the number of UV photons produced by stars to be sufficient to reionize the IGM. Such an estimate gives (e.g. Bromm & Loeb 2003)

$$J_{\text{bg}} \approx 4 \left( \frac{N_\gamma}{10} \right) \left( \frac{f_{\text{esc}}}{100\%} \right)^{-1} \left( \frac{1 + z}{11} \right)^3.$$

Here the number of UV photons required to ionize hydrogen is commonly taken to be $N_\gamma \sim 10$, and the escape fraction $f_{\text{esc}}$ is the fraction of ionizing photons (13.6eV) escaping from galaxies at high redshifts, which is expected to be close to unity (Whalen et al. 2004; see Fernandez & Shull 2010 for a recent discussion of the relevant $f_{\text{esc}}$ and for references to earlier works). From this equation, we find that the mean UV background at the time of reionization exceeds the critical flux $J_{\text{crit,H2}}$ by nearly an order of magnitude. While the radiation background will inevitably have spatial fluctuations, this implies that most halos collapsing in the early IGM, prior to reionization at $z \sim 10 - 20$, would be exposed to a super-critical flux and thus not able to cool below $T \sim 200K$. As a result, the emergence of low-mass PopIII.2 stars (or stars comparable in mass to those formed in the low-redshift universe) would be postponed until supernovae polluted the IGM with heavy elements, and metal-line cooling subsequently enabled gas clouds to reach temperatures near $T_{\text{CMB}}$.

There are several issues that could be important for the above conclusion, which we have glossed over in the discussion of our models for molecular shielding and one-zone spherical collapse. We next discuss some of these.

Uncertainty in the Column Density of the Collapsing Region. In our calculations, we have taken the diameter of the collapsing region to be of the order of the Jeans length. However, the effective size and column density will depend sensitively on the dynamical properties of the system, including bulk motions and internal velocity gradients in the gas, departures from spherical symmetry, etc.

In order to address this uncertainty quantitatively, we have performed two additional sets of runs for a halo with $T_{\text{vir}} \geq 10^4K$ (analogous to those in § 3.2.1). In the first, we increase the assumed size of the collapsing region by a factor of ten (i.e. to ten times the Jeans length $\lambda_\text{J}$). This increases the column densities by the same factor, and accordingly, $J_{\text{crit}}$ is larger by a factor of $\sim 3$ than the original result, due to more efficient self-shielding of H2 and – to a lesser extent – HD. Next, we investigated the cooling properties of a smaller collapsing core, with the assumed size reduced by a factor of ten, to 0.1$\lambda_\text{J}$. In this case, a new effect arises. Namely, for the values of $J_{21}$ at which the gas can (just) cool to around $T \sim 200K$, we find that direct HD dissociation is the dominant factor regulating the minimum temperature ultimately reached. In particular, switching HD dissociation off by hand in these cases decreases the gas temperature by a factor of $\sim 1.5$ at high number densities ($n \gtrsim 10^5$ cm$^{-3}$) for $J = 10^{-1}$. When the flux is weaker than this, artificially disabling the HD-dissociation has little effect; for these low fluxes, however, the suppression of HD–cooling is modest to begin with. As expected, the critical flux is decreased in this case because the smaller column densities leave both H2 and HD more susceptible to dissociation. In particular, we find a critical value of $J_{\text{crit}} \sim 10^{-1}$.

The Impact of 3-D Gas Dynamics on Self-Shielding. It is important to note that a full treatment of the three-dimensional dynamics of the system and the complexities inherent in radiative transfer is needed to solve the shielding problem exactly. Our calculation is based on a model of a uniform slab of gas with no internal velocity (or temperature) gradients. This is likely to be a poor approximation for a region undergoing runaway gravitational collapse, in which high gas velocities can produce significant Doppler shifts of the LW absorption bands of H2 and HD. In general, we expect this to
reduce the effective column densities, and the importance of shielding, compared to our calculations. This correction can be mitigated by the broadening of absorption lines at high column densities, which leads to line widths that are much larger than the average Doppler shift. In general, however, taking into account the possibility of Doppler shifts leads to the conclusion that our self-shielding results, and in turn the values quoted for $J_{\text{crit, HD}}$, are upper limits for both. This strengthens our argument above, namely, that most collapsing halos will see a super-critical flux.

Resonant Scattering of Incident LW Photons. An additional effect ignored by our self-shielding calculation is that after absorbing a LW photon, a fraction of molecules will decay directly back to the original ground state, as opposed to cascading through a series of lower energy decays as we implicitly assume. These photons are thus not eliminated, making the background flux stronger than we calculate. However, Glover & Brand (2001) estimate that in the case of H$_2$, such resonant scattering constitutes only a small fraction, 4-8%, of all LW absorption events (depending on the initial level populations; in particular, on theortho/para ratio). Hence this is a minor effect, which again makes our conclusions about the suppression of HD–cooling conservative.

Molecular Level Populations: Implications for Photo-dissociation Rates and the Critical Flux. As described in §3, our fiducial self-shielding calculations for HD and H$_2$ assume that all molecules are initially in the ro-vibrational and electronic ground states. In reality, molecules will occupy higher ro-vibrational states due to collisional excitation, and this can significantly increase the rates of photodissociation. In particular, we find that shielding is less effective (i.e. the shield factor is larger by a factor of a few) if we repeat our calculations, assuming LTE population distributions in the rotational levels ($J \neq 0$) within the ground electronic and vibrational state. (Data for the HD and H$_2$ energy levels were taken from Abgrall et al. 1982 and Dabrowski 1984 respectively.) Other studies have also noted that populations in higher vibrational levels ($v \neq 0$) can significantly increase the rates of photodissociation (e.g. Glover & Jappsen 2005, and references therein). Thus, if the effects of collisional excitation are taken into account, $J_{\text{crit, HD}}$ could be significantly lower than found above. The ro-vibrational distribution will be somewhat better approximated by the ground state model up to the critical densities ($n \gtrsim 10^4$ cm$^{-3}$ for H$_2$ and $n \gtrsim 10^6$ cm$^{-3}$ for HD). In our case, the fate of the collapsing clouds – whether it will ultimately cool to temperatures low enough for HD–cooling to become significant – is determined in the regime of somewhat lower gas densities, below those at which equilibrium H$_2$ populations are established, so that $J_{\text{crit}}$ values are likely closer to the upper end of the range.

Uncertainties in the Gas Phase Chemistry. The preceding discussion has focused on various uncertainties associated with photo-dissociation rates of H$_2$ and HD; however, the accuracy of any estimates of $J_{\text{crit, HD}}$ can only be as good as the accuracy of the underlying chemical rate coefficients. Considerable attention has been dedicated to uncertainties in both H$_2$ and HD chemistry and cooling, (e.g. Savin et al. 2004, Glover et al. 2006, Glover 2008, Glover & Abel 2008); accordingly, we restrict the discussion here to focus on two examples of thermal rate coefficients that have recently been updated, and how their revised values affect our results.

Two reaction rates that are crucial for determining the abundance of H$_2$, particularly in gas with a large initial ionization fraction, have been estimated to be uncertain by up to an order of magnitude (e.g. Glover & Abel 2008). These are the associative detachment channel for H$_2$ formation, and the mutual neutralization of hydride and protons (reactions 10 and 13 respectively in the compilation by SBH10):

$$ \text{H} + \text{H}^- \rightarrow \text{H}_2 + e^- \quad (16) $$

$$ \text{H}^+ + \text{H}^- \rightarrow \text{H} + \text{H}. \quad (17) $$

Both have been revisited recently and new thermal rate coefficients have been provided for reaction (10) by Kreckel et al. 2010 and for reaction (13) by Stenrup et al. 2009. As noted above, the formation of HD occurs primarily via the reaction pathway shown in equations 11-13 so in general, the fractional abundance of HD is proportional to that of H$_2$, justifying the emphasis here on uncertainties associated with the formation of H$_2$. In order to quantify how these recently updated rate coefficients impact our results, we have performed additional runs for each of the physical scenarios discussed in §3. The uncertainties these introduce into estimates of $J_{\text{crit, HD}}$ and the minimum temperature, $T_{\text{min}}$, reached when $J_{21}=0$, are summarized below.

We examine three published rate coefficients for the mutual neutralization reaction; the largest of these at all temperatures is that provided by GP98, hereafter $k_{13b}$. The rate used in our fiducial model ($k_{13b}$), originally provided by Dalgarno & Lepp (1987), is smaller than the others by up to an order of magnitude for $T \gtrsim 10^4$ K, and by a factor of several at lower temperatures. The value of the newest thermal rate coefficient, given by Stenrup et al. (2009), $k_{13c}$, lies between those of $k_{13b}$ and $k_{13b}$, at all temperatures in the regime we study. Using $k_{13b}$, we find the critical flux, $J_{\text{crit, HD}}$ is a factor of few lower than was found in each of the physical scenarios we have studied (see §3 note that this does not apply to the model of halos with $T_{\text{vir}} < 10^4$ K), and the minimum temperature is lowered by $\sim 30\%$ in the spherical collapse models. This is easily explained: when a large ionization fraction exists, reaction (13) competes with reaction (10) for the common reactant, H$^-$; thus, adopting a larger rate coefficient for reaction (13) leads to diminished abundance of, and less robust cooling by HD. Using the newest rate, $k_{13c}$, we find the critical flux is $\sim 30 - 40\%$ smaller than its original value for each physical scenario, and the minimum temperature is elevated by $\sim 20\%$ above that found previously in the spherical collapse models. (Note that the minimum temperature reached in the fossil HII region models does not depend on which rate coefficient is used for reaction 13.)

The effect of implementing the new rate for associative detachment is less dramatic; note, however, that the uncertainty associated with this rate coefficient has been reduced thanks to the recent study by Kreckel et al. (2010). Using the systematic uncertainty given by the authors, we implement the thermal rate at the ±1σ levels, and find the following ranges for the critical flux. In the fossil HII region:
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J_{crit, HD} = 3.85 \pm 0.15 \times 10^{-3} (n/10^2)$. In $T_{vir} > 10^4$K halos: $J_{crit, HD} = 3.7 \pm 0.2 \times 10^{-1}$ and $1.2 \pm 0.3 \times 10^{-2}$ when illuminated by T5 and T4 spectral types respectively. For a thorough discussion of how this new rate coefficient compares to previous calculations and its impact on H$_2$ chemistry, the reader is referred to Kreckel et al. (2010).

Two final notes on the chemical network are on order: first, we have not included in this study the formation of H$_2$ via a three-body reaction, by which metal–free gas can become fully molecular at $n \geq 10^8$ cm$^{-3}$, because our models do not include these high-density regimes. Lastly, as mentioned above, the primordial value of D/H varies in the literature by a factor of $\sim 2$, and this in itself may have consequences for the role of HD–cooling in metal–free gas.

**Fragmentation and Characteristic Protostellar Masses.** Finally, we emphasize that all our conclusions in this paper are based on the thermal history of a gas cloud, and how this is affected by a UV flux. In order to make realistic predictions for the fragmentation, and the ultimate sizes of stars forming in a collapsing halo, fully 3-D hydrodynamical simulations would be required. While robust HD–cooling (or lack thereof) could have a notable impact on the characteristic stellar masses in the earliest dwarf galaxies, the process of fragmentation is yet to be fully understood, and thus physical ingredients such as the minimum gas temperature may not directly translate into the actual mass of the protostar that ultimately forms (see, e.g., Clark et al. 2010 for recent results on fragmentation in metal-free gas, and in particular the importance of turbulence).

**5 SUMMARY**

We have demonstrated that HD–cooling in primordial gas can be suppressed by a relatively weak external LW background, with an intensity on the order of $J_{21} \sim 10^{-3} (n/10^{-2}$ cm$^{-3})$ in constant-density “fossil ionized” gas, and $J_{21} \sim 10^{-1}$ in shock– or photo–ionized gas collapsing into halos with virial temperatures greater than $\sim 10^4$K. These critical intensities are lower than the expected mean UV background at $z \sim 10–20$, suggesting that HD-cooling is likely unimportant in most proto-galaxies forming near and just prior to the epoch of reionization. We conclude that an “HD-mode” of star formation was not as prevalent as previously thought.

On a more technical note: we have also found that the negative feedback of the LW background is mediated via the abundance of molecular hydrogen, which is dissociated by the same radiation in its Lyman and Werner bands. Direct HD photo–dissociation is comparatively less important, although we find that in regimes of less effective self-shielding, it can regulate the minimum temperature of the gas. Finally, we have provided fitting formulae for the effects of HD and H$_2$ self-shielding, shielding of both species by HI, and shielding of HD by H$_2$, which we hope will be useful in other future studies.

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