Contribution of HD molecules in cooling of the primordial gas

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Abstract

We study the effects of HD molecules on thermochemical evolution of the primordial gas behind shock waves, possibly arised in the process of galaxy formation. We find the critical shock velocity when deuterium transforms efficiently into HD molecules which then dominate gas cooling. Above this velocity the shocked gas is able to cool down to the temperature of the cosmic microwave background. Under these conditions the corresponding Jeans mass depends only on redshift and initial density of baryons $M_J \propto \delta_c^{-0.5}(1+z)^{0.5}$. At $z > \sim 45$ HD molecules heat shocked gas, and at larger redshift their contribution to thermal evolution becomes negligible.

1 Introduction

Formation of stars is intimately connected with the ability of gas to cool. In the metal-free primordial medium the radiative cooling is mainly provided by molecular hydrogen and its isotope analogue HD. In the expanding universe H\textsubscript{2} and HD form after the epoch of recombination [1-5]. Due to a non-zero dipole moment and lower excitation energy HD molecules can efficiently cool gas at temperature $T \leq 200$ K, where the rate of H\textsubscript{2} cooling decreases sharply. If HD abundance is small, cooling of primordial gas stops practically at $T \leq 200$ K.

Thus, thermal evolution of the primordial gas at low temperature, and as a consequence characteristics of the first stars in the universe critically depend on the abundance of HD molecules. At present, an analysis of conditions when HD can be thermodynamically important in the primordial gas is absent. Conclusions about the role of HD molecules in a prestellar universe are contradictory. In particular, it is shown in [6] that HD cooling never dominates in a collapsing
spherical cloud. At the same time the authors [6-8] point out that HD cooling can be important in primordial clouds, although their calculations are restricted only by initial stages of the collapse. It is obvious though, that the abundance of HD crucially depends on thermal evolution of gas in the temperature range \( T > 500 \) K. The apparent contradiction about the role of HD is connected with differences in the initial conditions used in [1] from one side and in [6-8] from the other. In addition, the \( \text{H}_2 \) cooling function adopted in [1] is overestimated. Therefore, in order to make firm conclusions about the role of HD molecules in a prestellar universe it is necessary to investigate the efficiency of HD formation in a wider range of initial conditions.

It is known that formation of \( \text{H}_2 \) and HD molecules is largely boosted behind shock waves [10-13]. It is connected mostly with the fact that temperature and fractional ionization behind the shock waves increase, and as a consequence the rates of molecular reactions are enhanced. In a postshock gas cooled down to temperature \( \sim 10^4 \) the fraction of electrons remains sufficiently high, \( x \gtrsim 0.001 \), which favours rapid formation of \( \text{H}_2 \) molecules in the catalytic reactions with \( \text{H}^- \) ions. At such conditions \( \text{H}_2 \) fraction can reach \( \sim 10^{-2} \). Further cooling is mainly provided by \( \text{H}_2 \) molecules efficient in the temperature range \( 200 - 7000 \) K. When lower temperatures are reached, \( T \leq 200 \) K, deuterium begins to convert into HD molecules due to chemical fractionation [14, 15]. The contribution of HD cooling in energy losses increases when temperature decreases, and if it becomes dominant the gas temperature can fall down to several tens of degrees. One can expect that at least in a restricted range of shock parameters formation of HD molecules is as efficient as to provide such a predominance. We aim to study this possibility.

In Section 2 we describe a thermochemical model of a shocked gas; the results are presented in Section 3; in Section 4 discussion and in Section 5 summary are given. Throughout the paper we assume a \( \Lambda \)CDM cosmology with the parameters \((\Omega_0, \Omega_\Lambda, \Omega_m, \Omega_b, h) = (1.0, 0.71, 0.29, 0.047, 0.72)\) and deuterium abundance \( 2.62 \times 10^{-5} \) [16].

2 Molecular kinetics behind shock waves

In the absence of thermal conductivity and diffusion the thermochemical evolution of gas behind a shock wave can be described by a system of ordinary differential equations for a Lagrangian fluid element, which include equations of chemical kinetics

\[
\dot{x}_i = F(x_i, T, n) - D(x_i, T, n),
\]

and energy equation

\[
\dot{T} = \frac{2}{3} \sum_i \left[ \Gamma_i (x_i, T, n) - \Lambda_i (x_i, T, n) \right] + \frac{2}{3} \frac{T}{n} \dot{n},
\]
where \( x_i \) is the fraction of \( i \)-th species, \( F_i(x, T, n) \), \( D_i(x, T, n) \) are the corresponding formation and destruction rates, \( \Gamma_i(x, T, n) \), \( \Lambda_i(x, T, n) \) are the heating and cooling rates. Chemical kinetics of primordial gas include the following main species: \( \text{H}, \text{H}^+, \text{H}^- \), \( \text{He}, \text{He}^+, \text{He}^{++} \), \( \text{H}_2, \text{H}_2^+, \text{D}, \text{D}^+ \), \( \text{D}^- \), HD, HD\(^+\), e. \) The rates for collisional and radiative processes are taken from [4, 12], and for \( \text{D}^- \) ion from [3]. The energy equation accounts cooling processes connected with \( \text{H}, \text{He}, \text{He}^+, \text{He}^{++} \), such as collisional excitation and ionization, bremsstrahlung radiation, recombination, dielectronic recombination, molecular cooling by \( \text{H}_2 \) and HD, and Compton cooling. In the absence of external ionizing radiation the abundances of chemical species and radiative cooling are determined by collisions. Thus, the right-hand side of (1) and first term of the right-hand side of (2) are proportional to the gas density, and for convenience we can introduce the fluence \( \eta \) through

\[
d\eta = ndt, \tag{3}
\]

where \( t \) is time, \( n \) is number density; below the results are presented as functions of the fluence.

For the \( \text{H}_2 \) cooling functions we adopted the expressions given in [17], the HD cooling is taken from [18], the other rates are from [19]. In addition, the effects of interaction between molecules and the CMB photons are accounted [2, 15, 20] which imply that when gas temperature is close to the CMB temperature, \( \text{H}_2 \) and HD molecules are populated by the CMB photons, and then collisionally transfer the energy to kinetic temperature, thus heating the gas. Therefore, gas cannot cool lower than the CMB temperature. We assume that the gas temperature behind the front jumps and reach the value

\[
T_0 = \alpha^2 \frac{m_p v_c^2}{k} \simeq 1.2 \times 10^2 \alpha^2 \left( \frac{v_c}{1 \text{ km} \text{ c}^{-1}} \right)^2, \tag{4}
\]

where \( \alpha^2 = 3/16 \) is for a shock propagating in a static gas, and \( \alpha^2 = 1/3 \) is for a shock wave formed in a head-on collision of two flows (clouds) with equal velocities \( v_c \) [21]. Neglecting thermal conduction the evolution of each Lagrangian volume of gas behind the shock is isobaric [10, 12, 22], so that the density is described by

\[
n = \frac{P}{\mu kT}, \tag{5}
\]

where \( \mu \) is the average molecular weight.

### 3 Formation of HD behind shock waves

In the contemporary scenarios of structure formation in the universe the first protogalaxies form at the epoch \( z = 10 - 30 \). For specificity, we consider thermochemical evolution of baryons
behind a shock at the redshift $z = 20$. Formation of dark haloes (future protogalaxies) and their subsequent virialization are accompanied by shock waves in the baryon component. The duration of this process is close to the Hubble time $t_H(z)$ \cite{24}, so we restrict computations by $t_H(z)$, which means the ending redshift $z_e \simeq 12$ for the initial $z_i = 20$. One can expect that collisions of baryonic flows during the virialization of dark haloes result in considerable density variations. In order to study possible influence of such density variations on thermochemical evolution we conduct the calculations for a wide range of density in colliding flows: from the background to the virial value. As a characteristic value we adopt the virial density, $18\pi^2n_b(1 + z)^3$ (see e.g. \cite{24}), where $n_b$ is the background baryon density today, and consider the dependence of the thermochemical evolution on the initial gas density. Gas before the shock is assumed to be cold compared to the gas just after the front, so we consider strong shock waves.

HD molecules form efficiently at low temperature in the presence of sufficient fraction of molecular hydrogen through the reaction

$$D^+ + \text{H}_2 \longrightarrow \text{HD} + \text{H}^+.$$  

(6)

For this reason we briefly discuss formation and destruction of $\text{H}_2$ molecules behind shock fronts \cite{10,12,13,25}.

In the primordial gas $\text{H}_2$ forms in interactions of neutral hydrogen with $\text{H}^-$ and $\text{H}_2^+$ ions efficiently born at high temperature. As shock waves significantly increase temperature it enhances formation of $\text{H}_2$ and increases its abundance \cite{12}. It is known that HI cooling becomes inefficient at temperature $\lesssim 10^4$ K, and in the primordial gas only the molecular hydrogen can provide further cooling to lower temperature. One can estimate a minimum fraction of $\text{H}_2$ needed for effective cooling: the cooling time must be shorter then the Hubble time which condition fulfills when $\text{H}_2$ fraction becomes greater than the critical value $x_{\text{H}_2} = 5 \times 10^{-4}$ \cite{24}; an increase of $\text{H}_2$ abundance shortens the cooling time. In a shocked gas at temperature $\gtrsim 8 \times 10^3$ K collisions increase fractional ionization, and this further enhances formation of $\text{H}^-$, $\text{H}_2^+$ and $\text{H}_2$. Figures 1-3 show the evolutionary paths of the thermochemical state of a gas element behind the shock: the evolution begins at high temperature and follows a monotonous cooling accompanied by growing $\text{H}_2$ and HD fractions. It is seen that at high collisional velocities the electron fraction significantly increases at initial stages, which stimulates formation of $\text{H}^-$ ions and $\text{H}_2$ molecules and a strong decrease of temperature. The $\text{H}_2$ abundance grows rapidly in the temperature range $T \sim 10^3 - 10^4$ K, while at lower temperatures formation of $\text{H}_2$ practically exhausts \cite{25}. Already formed $\text{H}_2$ molecules provide further cooling down to $T \lesssim 150$ K deuterium rapidly
converts to HD molecules due to chemical fractionation (Fig. 4).

Fig. 5 presents the dependence of electron, $H_2$ and HD fractions on the fluence $\eta = \int ndt$ for several values of the shock velocity. Note that for the shock waves with $v_s \geq 3.5\alpha^{-1}$ km s$^{-1}$ the final abundance of $H_2$ is greater than the limit $5 \times 10^{-4}$, and as a consequence the gas behind the shock can lose significant fraction of its thermal energy in one Hubble time. Since larger shock velocity corresponds to higher temperature, the maximum density behind the shock increases with the velocity $\rho \propto v_s^2$ (eqs. 4 and 5). In Fig.5 this corresponds to larger fluence. It is obvious, that the characteristic time of the thermal evolution decreases as $\propto v_s^{-2}$. For $v_s \simeq 4.6\alpha^{-1}$ km s$^{-1}$ $H_2$ fraction equals $\sim 7 \times 10^{-4}$ and becomes sufficient for cooling down to $T \simeq 130$ K; HD fraction at these conditions is $4 \times 10^{-7}$. Further increase of the shock velocity results in an increase of molecular fractions and a decrease of temperature on a shorter time, with the dominant cooling provided by HD molecules (Fig.6). Equating the cooling rates from $H_2$ and HD one can estimate the critical temperature below which the contribution of HD into thermodynamics becomes dominant. For the adopted cooling functions it occurs at $T_{cr} \simeq 130$ K. For the shock wave velocity $\sim 4.6\alpha^{-1}$ km s$^{-1}$ gas cools down to this limit, and for larger velocities temperature falls below $T_{cr}$ where the HD cooling dominates.

In the velocity range $4.6\alpha^{-1} \lesssim v_s \lesssim 8.7\alpha^{-1}$ km s$^{-1}$ the initial temperature behind the shock is insufficient for collisional ionization, and in the subsequent evolution the electron fraction can only decrease (Figs.1 and 5). At such conditions $H_2$ and HD abundances increase with velocity only because the reaction rates grow with temperature. As seen in Fig.2 for shock velocities in this range the maximum fraction of $H_2$ is approximately equal to $x_{H_2} \simeq 8 \times 10^{-4}$. This is enough for an efficient formation of HD molecules and successful cooling down to $T \leq 130$ K. At $v \gtrsim 7\alpha^{-1}$ km s$^{-1}$ the HD fraction becomes sufficient for cooling down to the CMB temperature $T_{CMB} = 2.7(1 + z)$: due to the strong emission in rotational lines of HD gas temperature falls to several tens, $\sim 30$ K, approaching $T_{CMB}(z)$ at a given redshift (Fig.5). This is because HD molecules provide an efficient exchange of energy between the CMB and baryons through absorption of CMB photons and subsequent collisional de-exitation [2, 15, 20]. It is obvious that similar picture is valid at all redshift, and the final temperature of cold baryons is $T_{min} \simeq T_{CMB}$.

For velocities $v_s \gtrsim 9.2\alpha^{-1}$ km s$^{-1}$ gas temperature behind the shock becomes greater than $10^4$ K, which results in an increase of fractional ionization immediately after the gas element crosses the shock front: for $v_s = 10.4\alpha^{-1}$ km s$^{-1}$ $x_e$ increases by factor of 2, and for $v_s \gtrsim 11.6\alpha^{-1}$ km s$^{-1}$ more than an order (Fig.1 and 5). At such conditions chemical kinetics changes qualitatively – the enhancement of $H_2$ formation is caused in this case by the two
factors: increasing reaction rates and a higher ionization fraction, resulting in more frequent catastrophic processes $H + e \rightarrow H^{-1}$, $H^{-1} + H \rightarrow H_2 + e$. The corresponding evolution of $x_e(t)$, $x_{H_2}(t)$ and $x_{HD}(t)$ looks qualitively different as seen in Fig. 5: while for $v_s < 9.2 \alpha^{-1}$ km s$^{-1}$ an increase of velocity by 1 km s$^{-1}$ produces insignificant changes in $x_{H_2}(t)$ and $x_{HD}(t)$, for greater velocities such an increase results in a considerable (half order of magnitude) increase of $x_{H_2}(t)$ and $x_{HD}(t)$. Thus, $x_{H_2}(t)$ and $x_{HD}(t)$ fractions at equal temperatures are higher for larger velocities (Figs. 2 and 3). For lower velocities the evolutionary paths $x_{H_2}(T)$ and $x_{HD}(T)$ for different $v_s$ practically coincide at temperature $T \leq 10^3$ K. One should stress, that in the considered range of velocities $H_2$ molecules form primarily through $H^-$ ions, the contribution from $H_2^+$ ions is as a rule negligible.

Thus, for velocities $v \geq 4.6 \alpha^{-1}$ km s$^{-1}$ HD molecules behind shock waves provide lower temperatures than $H_2$ can do. It is worth noting that at $z \sim 45$ the CMB temperature is higher than the critical value $T_{cr}$ at which HD cooling dominates. Therefore, under these conditions HD molecules can only heat gas, and at larger redshifts become unimportant.

Everywhere above we adopted gas density in colliding flows equal to the virial value at the corresponding redshift. However, one can assume that in the process of merging of haloes a fraction of baryonic mass can be lost. In the intergalactic medium such "separated” baryonic flows can greatly expand, and their final density depends on collision velocity $v_c$, masses of the merging haloes, details of separation and so on. Subsequently such baryonic clumps can collide with gaseous components of other haloes or with each other. In these conditions the thermal evolution differs from that of denser baryonic flows. Let us consider how the thermochemical evolution depends on the density. Fig. 7 shows the temperature and the HD fraction versus the density for several shock velocities at two redshifts. It is clearly seen that at $z = 20$ and in the low velocity range $v \leq 5.8 \alpha^{-1}$ km s$^{-1}$ only for densities close to the virial value gas temperature drops below the critical value where contribution from HD dominates. However, for higher velocities HD cooling remains efficient even for densities of one order of magnitude lower than the virial value. At $v \simeq 5.8 \alpha^{-1}$ km s$^{-1}$ and the density close to the virial value only $\simeq 0.25$ of deuterium converts in HD, however it becomes sufficient to cool the gas down to the CMB temperature. For higher velocities this can occur for several times lower densities than the virial value. Collisions with higher velocities $v \geq 11.6 \alpha^{-1}$ km s$^{-1}$ change $H_2$ kinetics: formation of $H_2$ becomes more efficient due to significant increase of fractional ionization behind the front, and behaves similar to the collisions with virial density at $v_s \gtrsim 10.4 \alpha^{-1}$ km s$^{-1}$ shown in Figs. 1 and 5. These features are seen in Fig. 7. In general, one can conclude that HD molecules can
also play a significant role in cooling of baryonic flows of low density.

4 Discussion: formation of protostellar fragments

Birth of stars is always accompanied with shock waves. This is unconditionally true for the first stars in the universe. The origin of shock waves can be connected both with the formation of the first protogalaxies in merging flows, and with supernovae explosions in already formed galaxies. Formation of the first protogalaxies implies separation of highly overcritical density perturbations from the Hubble expansion and a predominantly one-dimensional compression \[26, 27\]. This is a source of shock waves in baryonic component. Similar processes take place in the hierarchical scenario of structure formation, where massive objects form in collisions and following mergings of less massive haloes. These processes can be treated as collisions of the gas and dark matter flows. A collisionless dark matter reaches the virial state apparently through the violent relaxation, while in gas component shock waves form. The shock wave velocity depends on mass of a forming protogalaxy: the velocity amplitude in a perturbation of mass \(M\) is close to the value

\[ v_c = \sqrt{3} \sigma, \]  

(7)

where \(\sigma\) is the one-dimensional velocity dispersion \[28\]

\[ \sigma^2 = \frac{GM}{2R}. \]  

(8)

Thus, the parameters of the shock waves are determined by the total mass of matter involved in motion, by the redshift at which the object forms, and so on. The efficiency of HD formation is sensitive to these parameters. Therefore, one can expect that the characteristics of stellar population vary in galaxies of different mass. As the maximum abundance of HD depends on the shock velocity, and HD molecules cool the gas to much lower temperature than \(\text{H}_2\) molecules do, a typical mass of protostellar molecular clouds is expected to decrease with increasing mass of a forming galaxy \[29\].

Shock waves in the epoch of galaxy formation can be connected with explosions of the first supernovae. In these events much more powerful shock waves form: typical velocities can be greater \(\gtrsim 100\ \text{km s}^{-1}\), the corresponding temperature behind the front is \(\gtrsim 2.8 \times 10^5\ \text{K}\). At radiative stages when the gas temperature reaches \(\lesssim 10^4\ \text{K}\), the \(\text{H}_2\) fraction becomes sufficiently high \(\gtrsim 5 \times 10^{-3}\) \[12, 30\] due to high ionization fraction at the preceding stages. As a consequence, the gas temperature definitely falls to the lower values at which the cooling
is essentially determined by HD molecules. In these conditions fragmentation of an expanding shell can occur [31].

Due to isobaric compression the gas density behind the shock increases considerably compared to the initial value. For instance, for the velocity \( v_c \geq 7 \alpha^{-1} \) km s\(^{-1} \) the initial temperature is \( T \geq 5.8 \times 10^3 \) K [4], and when the gas cools down to \( T_{\text{CMB}} \simeq 2.7(1 + z) \), its density increases more than 200 times. At such conditions fragmentation and formation of stars become possible behind the shock [32]. Gravitationally unstable fragments can give rise to protostars or protostellar clusters. It follows that when cooling is determined by HD molecules, formation of low mass protostellar clouds becomes possible [33, 34]. Indeed, under these conditions the gas temperature falls down to \( \sim 2.7(1 + z) \) K which at \( z = 20 \) is 4 times smaller than can be provided only by H\(_2\) molecules. The Jeans mass \( M_J \simeq 30T^{3/2}n^{-1/2}M_\odot \) behind the front is \( M_J \simeq 15T^2n_0^{-1/2}T_0^{-1/2}M_\odot \), where \( n_0 \), the gas density in a flow (a cloud) before collision, \( T_0 \) is the temperature at the shock; here density at the front is taken 4\( n_0 \) as for strong shock waves.

If we assume that gas density in flows (clouds) before collision is equal to the virial value (see e.g. [24]), \( n_0 = 18\pi^2n_b(1 + z)^3 \), then for velocities \( v_c \geq 7 \alpha^{-1} \) km s\(^{-1} \) (or initial temperature \( T_0 \geq 5.8 \times 10^3 \) K) the Jeans mass is

\[
M_J \simeq 2.4 \times 10^5 M_\odot \left( \frac{1 + z}{T_0\delta_c} \right)^{0.5} = 7.2 \times 10^3 M_\odot \left( \frac{\alpha v}{1 \text{ km s}^{-1}} \right)^{-1} \left( \frac{\delta_c}{18\pi^2} \right)^{-0.5} \left( \frac{1 + z}{20} \right)^{0.5}
\]

where \( \delta_c \) is the ratio of gas density before collision to the background baryonic density. At the same time, when cooling is determined only by H\(_2\) molecules the typical gas temperature is of \( \sim 200 \) K, and the corresponding Jeans mass \( \sim 13.5[(1 + z)/20]^{-2} \) times exceeds the value given by [9]

\[
M_J \simeq 1.3 \times 10^9 M_\odot \left( \frac{1}{T_0\delta_c(1 + z)^3} \right)^{0.5} = 10^5 M_\odot \left( \frac{\alpha v}{1 \text{ km s}^{-1}} \right)^{-1} \left( \frac{\delta_c}{18\pi^2} \right)^{-0.5} \left( \frac{1 + z}{20} \right)^{-1.5}
\]

In other words, the question of how massive are the fragments formed behind shock fronts depends on whether the cooling is determined by H\(_2\) or HD molecules. The density of the fragments is \( \geq 10 - 300 \) cm\(^{-3} \) depending on the redshift and the initial temperature. Subsequent collapse is isothermal until the fragment becomes opaque in H\(_2\) and HD lines, which takes place at the density \( \sim 10^9 - 10^{10} \) cm\(^{-3} \). At this stage, if the cooling is dominated by HD molecules, the Jeans mass is \( M_J \sim 30T_{\text{CMB}}^{3/2}n^{-1/2}M_\odot \sim 10^{-3}(1 + z)^{3/2}M_\odot \) [29], however when HD is underabundant the Jeans mass can be 2-3 orders greater [35]. Further evolution is determined by the accretion of gas onto the central core [36, 37]. If the accretion rate is below the Eddington limit, the mass of a forming star is comparable to the initial mass of a protostellar cloud, in the opposite case it can be much lower [35, 36]. Thus, one can expect that a typical mass of the
first stars born in protogalaxies of higher masses (corresponding to higher collisional velocities) is shifted towards the lower end due to cooling by HD molecules.

It is readily seen that since the overall thermal evolution of low density flows differs from that of higher densities, the final value of the Jeans mass and its dependence on redshift will differ from the above value. Fig.7 shows the Jeans mass versus the gas density in the flow. In the range of collisional velocities $5.8 \alpha^{-1} \leq v_c < 8.6 \alpha^{-1} \text{ km s}^{-1}$ only flows with the initial density very close to the virial can have Jeans mass $M_J$ smaller than $10^4 M_\odot$, which may correspond to the mass of a protostellar cloud. However for $v \geq 8.6 \alpha^{-1} \text{ km s}^{-1}$ the Jeans mass becomes $\leq 10^4 M_\odot$ for the initial density 4 times lower than the virial. As mentioned above, for higher velocities gas cools down to the CMB temperature, and the Jeans mass is $\leq 10^3 M_\odot$, what is seen also from (9) – on Fig.7 flat parts of the lines for the velocity $\geq 8.6 \alpha^{-1} \text{ km s}^{-1}$ reflects this circumstance. Thus, the Jeans mass is considerably higher than (9) only for flows with a low collisional velocity and a low density. High-velocity collisions $v_c \geq 8.6 \alpha^{-1} \text{ km s}^{-1}$ provide cooling down to the temperature $T \simeq T_{\text{CMB}}$ even for low density flows.

Let us consider collision of flows whose density is equal to the background value, i.e. $\delta_c \simeq 1$, $\rho/\rho_{\text{vir}} \simeq 6 \times 10^{-3}$. It is seen from Fig.7 that even for high-velocity collisions $v_c = 11.6 \alpha^{-1} \text{ km s}^{-1}$ gas cannot cool sufficiently in one Hubble time, and the Jeans mass is quite high: $\sim 10^6 - 10^7 M_\odot$. Moreover, the free-fall time for such low densities is greater than the comoving Hubble time. Under these conditions baryonic objects cannot be formed. However, further increase of the collisional velocity, $v_c > 11.6 \alpha^{-1} \text{ km s}^{-1}$, makes the gas behind the shock able to cool down to the temperature $\leq 1000 \text{ K}$ during one Hubble time. For instance, for low density flows collided with the velocity $v_c \simeq 19.2 \alpha^{-1} \text{ km s}^{-1}$ the final temperature behind the shock is $\sim 200 \text{ K}$, and can reach lower values for higher velocities. Under these conditions HD molecules will dominate in gas cooling, and the Jeans mass becomes as small as $\sim 7 \times 10^4 M_\odot$.

## 5 Conclusions

The influence of HD molecules on the thermochemical evolution of the primordial gas behind shock waves possibly formed during the epoch of galaxy formation has been studied.

1. We showed that deuterium converts efficiently to HD molecules and the contribution of HD to cooling becomes dominant for the shock waves with velocities $\gtrsim 4.6 \alpha^{-1} \text{ km s}^{-1}$ ($\alpha \simeq 0.5$). Behind such shock waves the conditions are favourable for fragmentation and, as a consequence, for formation of protostellar clusters.
2. For shock velocities $\gtrsim 7\alpha^{-1}$ km s$^{-1}$ gas is able to cool down to the CMB temperature. Under these conditions Jeans mass depends only on the redshift and the initial density:

$$M_J \lesssim 2.4 \times 10^5 M_\odot (1 + z)^{0.5} (T_0 \delta_c)^{-0.5},$$

for virial haloes ($\delta_c = 18 \pi^2$) at $z = 20$ this corresponds to $M_J \lesssim 10^3 M_\odot$.

3. At $z \gtrsim 45$ the CMB temperature is close to the critical value $T_{cr}$, at which the contribution from HD molecules to the total cooling is comparable to that from H$_2$. At these conditions HD molecules begin to heat gas, and at higher redshifts become unimportant in thermal history of baryons.

4. For densities of colliding flows smaller than the virial value the efficiency of HD molecule formation decreases. In particular, at $z = 20$ gas temperature behind the shock with $v \sim 5.8\alpha^{-1}$ km s$^{-1}$ drops substantially only for a density close to the virial value. However, for the shock velocities $\sim 8.6\alpha^{-1}$ km s$^{-1}$ HD molecules are important in cooling for densities of 2-3 times lower than the virial value. For $v \sim 11.6\alpha^{-1}$ km s$^{-1}$ HD cooling is effective for densities close to the background value, and almost all deuterium converts to HD for collisions of less dense than if the flows were virial. For the gas density equal to the background value and for the velocity $v \gtrsim 19.2\alpha^{-1}$ km s$^{-1}$ temperature drops to $\leq 200$ K and HD molecules begin to dominate radiative cooling.

References

[1] S. Lepp, J.M. Shull, Astrophys. J. 280, 465 (1984)

[2] D. Puy, G. Alecian, J. Le Bourlot, et al., Astron. and Astrophys. 267, 337 (1993)

[3] F. Palla, D. Galli, J. Silk, Astrophys. J. 451, 44 (1995)

[4] D. Galli, and F. Palla, Astron. and Astropys. 335, 403 (1998)

[5] P.C. Stancil, S. Lepp, A. Dalgarno, Astrophys. J. 509, 1 (1998)

[6] E. Bougleux, D. Galli, Monthly Notes Roy. Soc., 288, 638 (1997)

[7] D. Puy, and M. Signore, NewA 2, 299 (1997)

[8] D. Puy, and M. Signore, NewA 3, 247 (1998)

[9] F. Palla, Proceedings of Star Formation 1999, ed. T. Nakamoto, Nobeyama Radio Observatory, p.6 (1999)
[10] A. A. Suchkov, Yu. A. Shchekinov, M. A. Edelman, Astrophysics, 18, 360 (1983)

[11] M.-M. Mac Low, J.M. Shull, Astrophys. J. 302, 585 (1986)

[12] P.R. Shapiro, H. Kang, Astrophys. J. 318, 32 (1987)

[13] H. Kang, P.R. Shapiro, Astrophys. J. 386, 432 (1992)

[14] P. M. Solomon, N. J. Woolf, Astrophys. J. 180, 89 (1973)

[15] D. A. Varshalovich, V. K. Khersonskii, SvAL, 2, 227 (1976)

[16] D. N. Spergel, L. Verde, H.V. Peiris et al., Astrophys. J. Suppl. 148, 175 (2003)

[17] D. Hollenbach and C.F. McKee, Astrophys. J. Suppl. 41, 555 (1979)

[18] D. Flower, Monthly Notes Roy. Soc., 318, 875 (2000)

[19] R. Cen, Astron. J. Suppl. 78, 341 (1992)

[20] D. Galli, and F. Palla, Planetary and Space Sci. 12-13, 1197 (2002)

[21] J. Smith, Astrophys. J. 238, 842 (1980)

[22] P. Anninos, M. Norman, Astrophys. J. 460, 556 (1996)

[23] Ya. B. Zeldovich, I.D. Novikov, Relativistic astrophysics. v.2 - The structure and evolution of the universe, University of Chicago Press (1983)

[24] M. Tegmark, J. Silk, M.J. Rees, et al., Astrophys. J. 474, 1 (1997)

[25] S.P. Oh, Z. Haiman, Astrophys. J. 569, 558 (2002)

[26] C. Lin, L. Mestel, F. Shu, Astrophys. J. 142, 1431 (1965)

[27] Ya. B. Zeldovich, Astron. & Astrophys. 5, 84 (1970)

[28] A. Blanchard, D. Valls-Gabaud, G.A. Mamon, Astron. and Astrophys., 264, 365 (1992)

[29] E. O. Vasiliev, Yu. A. Shchekinov, Astr. Rept. 49, 587 (2005)

[30] A. Ferrara, Astrophys. J., 499, L17 (1998)

[31] E. T. Vishniac, Astrophys. J., 274, 152 (1983)

[32] M. Yamada, R. Nishi, Astrophys. J. 505, 148 (1998)
Note added in manuscript 2005 July 26. - After acceptance of this paper we have been informed about the paper by A. Lipovka, R. Núñez-López, and V. Avila-Reese (MNRAS, 2005, in press, astro-ph/0503682), where new calculations of the HD cooling function are reported. In the temperature range of interest ($T < 10^3$ K) this function coincides with that given in [18], while at higher temperatures, where Lipovka et al predict an order of magnitude enhanced HD cooling rate, the abundance of HD is too low to contribute.
Figure 1: The evolutionary paths connecting fractional ionization and gas temperature behind
shocks in collisions with velocities 2.3, 3.5, 4.6, 5.8, 7, 8, 9.2, 10.4, 11.6 α⁻¹ km s⁻¹ – from top
to bottom; initial points of the evolution are marked by filled circles.
Figure 2: The evolutionary paths connecting variations of temperature and H$_2$ concentration for the same velocities as in Fig. 1 (left to right). The vertical line depicts the critical value $5 \times 10^{-4}$ needed for baryons to cool in one comoving Hubble time [21].
Figure 3: The evolutionary paths for the abundance of HD molecules (see Fig. 1).
Figure 4: The relative contribution of radiative losses in the lines of H$_2$ and HD into the total cooling (see Fig.1). Squares mark the initial points, circles – the final points of the evolution for the velocities 2.3, 3.5, 4.6, 5.8, 7, 8, 9.2, 10.4, 11.6 $\alpha^{-1}$ km s$^{-1}$.
Figure 5: Ionization, $\text{H}_2$, HD fractions and temperature behind the shock front versus $\eta$ for the velocities 2.3, 3.5, 4.6, 5.8, 7, 8, 9.2, 10.4, 11.6 $\alpha^{-1}$ km s$^{-1}$. Circles on temperature lines mark the final points of the evolution.
Figure 6: The relative contribution of radiative losses in the lines of $H_2$ and HD into the total cooling (see Fig.5). Filled ($H_2$) and open (HD) circles mark final points of the evolution for velocities 2.3, 3.5, 4.6, 5.8, 7, 8, 9.2, 10.4, 11.6 $\alpha^{-1}$ km s$^{-1}$ (left to right).
Figure 7: Temperature, HD fraction and Jeans mass reached behind the shock fronts with the velocities 2.9, 5.8, 8.6, 11.6 km s$^{-1}$ for two redshifts: $z = 20$ – solid, $z = 15$ – dashed lines. Shaded area on the top panel shows the region where the HD cooling prevails. The density in units of the virial value for $z = 20$ is shown at the upper axis.