

Cosmic rays and the primordial gas

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ABSTRACT

One of the most outstanding problems in the gravitational collapse scenario of early structure formation is the cooling of primordial gas to allow for small mass objects to form. As the neutral primordial gas is a poor radiator at temperatures $T \leq 10^4$ K, molecular hydrogen is needed for further cooling down to temperatures $T \sim 100$ K. The formation of molecular hydrogen is catalyzed by the presence of free electrons, which could be provided by the ionization due to an early population of cosmic rays. In order to investigate this possibility we developed a code to study the effects of ionizing cosmic rays on the thermal and chemical evolution of primordial gas. We found that cosmic rays can provide enough free electrons needed for the formation of molecular hydrogen, and therefore can increase the cooling ability of such primordial gas under following conditions: A dissociating photon flux with $F < 10^{-18}$ erg cm⁻² Hz⁻¹ s⁻¹, initial temperature of the gas $\sim 10^3$ K, total gas number densities $n \geq 1$ cm⁻³, Cosmic ray sources with $\dot{\epsilon}_{CR} > 10^{-33}$ erg cm⁻³ s⁻¹.

Key words: cosmic rays – astrochemistry.

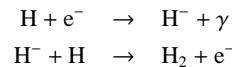
1 INTRODUCTION

In the commonly adopted theory for structure formation, primordial density perturbations grow through gravitational Jeans' instability and eventually form halos in whose potential wells the observable baryonic matter gathers. During contraction, the gas develops shocks and gets reheated to a temperature at which pressure support can prevent further collapse. Once the gas has virialized in the potential wells of pre-existing dark matter halos, additional cooling is then required to further collapse the gas and form luminous objects.

Line cooling, in which the radiative de-excitation of atoms leads to the emission of photons, is the most important cooling mechanism for a primordial gas (predominantly made of hydrogen and helium) at temperatures $T > 10^4$ K. At lower temperatures though, primordial gas is a very poor radiator (Shapiro & Kang 1987) and in the absence of elements with lower excitation energies, such as metals, line cooling becomes ineffective (Galli & Palla 1998). In the standard cosmological hierarchical scenario for structure formation the objects which form first are predicted to have masses corresponding to virial temperatures $T_{vir} < 10^4$ K (for a review see Ciardi & Ferrara 2005). Thus these objects, once virialized, cannot cool and further collapse via atomic line cooling.

The most efficient coolant for a primordial gas at such temperatures is molecular hydrogen, because it has additional rotational and vibrational degrees of freedom and therefore is able to cool the gas down to temperatures $T \sim 100$ K. For this reason molecular hydrogen is believed to play an important role in the formation of stars or small-mass galaxies from a metal-free gas.

Therefore, it is of great interest to get a firm picture of the primordial chemistry and of all the effects that might lead to formation or destruction of molecular hydrogen in metal-free gas. At redshifts $z \leq 110$ molecular hydrogen is predominantly formed by the gas phase reactions



in which electrons act as a catalyst (Dalgarno & Lepp 1987). Thus, the formation of molecular hydrogen requires free electrons to be abundant at relatively low temperatures ($T \leq 10^4$ K).

In a post recombination universe the gas is mainly neutral with a residual fraction of free electrons which give rise to the formation of traces of molecular hydrogen (Galli & Palla 1998). Nevertheless, this primordial abundance is not enough to trigger structure formation (Hirata & Padmanabhan 2006; Abel et al. 1997; Tegmark et al. 1997; Haiman & Loeb 1997). Partial ionization of hydrogen and helium increases the abundance of free electrons and promotes the formation of molecular hydrogen. While UV photons can fully ionize such species and, in the absence of neutral hydrogen, prevent the formation of H₂, x-rays only produce a partial ionization and promote molecular hydrogen formation. In the past, several authors have investigated the influence of x-rays on the H₂ chemistry (e.g. Glover & Brand (2003); Haiman et al. (2000)).

Recently much work has been published on the effect on primordial chemistry of high energetic cosmic rays arising from the decay of massive dark matter particles (e.g. Shchekinov & Vasiliev 2004; Ripamonti et al. 2006). Shchekinov & Vasiliev (2004) pointed out that ultra high energetic cosmic rays (UHECR), arising from decaying super heavy dark matter particles with masses

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$M_X \geq 10^{12}$ GeV may have a strong effect on the chemical evolution of the medium. Those high energy cosmic rays are believed to be converted into UV photons through electromagnetic cascades which would partially ionize hydrogen and eventually lead to the formation of molecular hydrogen. The authors showed that in the presence of UHECR the early luminous objects are an order of magnitude less massive and form earlier in comparison to the predictions of the standard recombination history.

Cosmic rays (CR) themselves can be an alternative source of partial ionization. Unlike photons, cosmic ray particles can ionize neutral atoms many times as they move through the medium. In addition, in each ionizing collision the cosmic ray particles impart only a small fraction of their overall kinetic energy to the ejected electron (Mannheim & Schlickeiser 1994; Spitzer & Scott 1969). Therefore cosmic rays are expected to heat the medium much less than photons with comparable energies. There are several suggestions about possible cosmic ray sources in the early universe. Decaying primordial black holes, topological defects, the very early supernovae, super massive particles or structure formation shocks are some of these (Biermann & Sigl 2001; Stanev 2004; Pfrommer et al. 2006).

In this paper we will investigate whether an early population of cosmic rays can trigger molecular hydrogen formation and contribute to the process of small scale structure formation. This will be done by coupling in a self-consistent way the spectral evolution of a cosmic ray population with the chemical evolution of a primordial gas. In Section 2 and 3 we describe the chemical evolution of the gas and the evolution of the cosmic ray spectrum respectively. In Section 4 and 5 we describe how cosmic rays interact with the ambient matter and by which reactions they influence the primordial chemistry. The method and the code developed during this work will be described in Section 6. Finally, Section 8 contains a discussion on the results which will be summarized in Section 9.

2 PRIMORDIAL CHEMISTRY

As discussed in the Introduction the basic idea of this work is to study the effect of cosmic rays on a gas consisting of different primordial chemical species. Among others, we want to investigate the relevance of cosmic rays for early structure formation, which takes place in an almost metal free universe between redshift $z \sim 40$ and $z \sim 10$. We therefore consider only the chemistry of primordial elements, hydrogen, H, helium, He and deuterium, D. These three species interact via a complicated network of chemical reactions, which changes the overall chemical state of the gas.

According to Spitzer (1978) the velocity distributions of the gas particles in the density regime considered in this work (1 to 10^4 cm⁻³) are always close to a Maxwellian equilibrium distribution. This allows to describe the thermal state of this multi-component gas with just one single kinetic temperature T for all particles.

Although the velocity distributions of the particle species are close to that in thermal equilibrium, the level population of the different species does not correspond to thermal equilibrium. In the density regime considered here though, the coronal limit can be applied. This allows to treat all particle species, including molecular hydrogen, in their ground states as long as only moderate UV fields with fluxes up to $\sim 10^{-15}$ erg cm⁻² s⁻¹ Hz⁻¹ are present (Abel et al. 1997; Shull 1978).

Given the above approximations, a simplified approach can be used to describe numerically the chemical and thermal evolution

of the gas. The chemical evolution of a gas is governed by inelastic collisions that change the number densities of interacting species by creating or destroying chemical compounds. The equation which governs the number density evolution is most generally given as:

$$\frac{dn_i}{dt} = \sum_j \sum_k \alpha^i k_{jk}^i(T) n_j n_k + \sum_l \beta^i \lambda_l^i n_l - n_i \frac{d \ln V}{dt}. \quad (1)$$

Here the subscripts i, j, k and l denote the different particle species, and the quantities $k_{jk}^i(T)$ and λ_l^i are the rates for the chemical reactions that create or destroy particles of type i (reference to the used rates is given in Appendix B). α^i and β^i are the stoichiometric coefficients that account for the number of particles of type i that are created or destroyed in each reaction. The last term in equation (1) describes the change in particle number density due to the evolution of the volume V .

Whereas the temperature evolution of the gas is described by:

$$\frac{dT}{dt} = \frac{2(\Gamma - \Lambda)}{3nk_B} - \frac{2}{3} \frac{d \ln V}{dt} T, \quad (2)$$

where $n = \sum_i n_i$ is the total number density and Γ and Λ are the heating and cooling functions respectively (Appendix A). The first term on the right hand side of equation (2) describes the net thermal heat input to the medium, while the second term describes the work done by compression or expansion of the gas. Note that here we assume that the gas behaves as an ideal mono-atomic gas (Spitzer 1978). Effects of thermal conduction are neglected in equation (2), which is appropriate for the density and temperature range considered here (Spitzer 1978).

3 COSMIC RAY SPECTRAL EVOLUTION

It is well known that radiation like cosmic rays can ionize neutral atoms and deeply influence the chemical evolution of a medium. Since protons are the dominant cosmic ray species at least in our Galaxy (Pfrommer et al. 2006), here we will only consider the cosmic ray protons. This is a fair assumption as nucleosynthesis predicts $\approx 93\%$ of all baryon particles in the universe to be protons. Therefore the dominant species emitted by some early cosmic ray accelerator should also be protons. However, a small fraction of helium might be present in the early cosmic radiation. These α -particles can simply be treated as four protons and hence be absorbed in the proton spectrum (Enßlin et al. 2006).

Since the ionization cross section of hydrogen has a maximum at proton impact energies ≈ 25.0 keV, it is necessary to find an adequate representation of the cosmic rays at those low energies. In addition, their original spectrum will be modified due to the energy losses which cosmic rays experience in the frequent interactions with particles of the ambient medium. As no measurement of low energetic cosmic rays is available and the cosmic ray ionization rate depends on the spectrum, we need to model the low energy spectrum and its time evolution theoretically.

In the following we will define some variables useful for our calculations. It is convenient to introduce the dimensionless momentum:

$$p = \frac{p_{CR}}{m_p c}, \quad (3)$$

where p_{CR} is the momentum of the cosmic ray proton and m_p is the proton mass. In addition, we can express the kinetic energy T_p as:

$$T_p(p) = \left(\sqrt{1 + p^2} - 1 \right) (m_p c^2) \quad (4)$$

and the dimensionless velocity β as:

$$\beta = \frac{v}{c} = \frac{p}{\sqrt{1+p^2}} \quad (5)$$

where v is the particle velocity.

With this notation the spectral evolution equation of the cosmic ray proton number density $n(p, t)$ can be written as follows:

$$\frac{\partial n(p, t)}{\partial t} + \frac{\partial \dot{p}(p, t)n(p, t)}{\partial p} = Q(p, t) - \frac{n(p, t)}{\tau(p, t)}, \quad (6)$$

where the dot denotes the derivative with respect to time, $Q(p, t)$ is a source function for the cosmic ray protons and $\tau(p, t)$ is a typical loss time for cosmic ray particles from the volume under consideration.

Under the assumption that the injected spectrum obeys a power law with some spectral index s in momentum space, the source function can be written as:

$$Q(p, t) = \frac{\dot{\epsilon}_{CR}}{m_p c^2 \kappa(s, p_0)} p^{-s} \Theta(p - p_0), \quad (7)$$

where $\dot{\epsilon}_{CR}$ is the change of total cosmic ray energy density with respect to time, $\kappa(s, p_0)$ is a normalization depending on the spectral index s , $\Theta(x)$ is the Heaviside function and p_0 is a lower momentum cutoff of the injected spectrum. The value of $\kappa(s, p_0)$ can be calculated as (Enßlin et al. 2006):

$$\kappa(s, p_0) = \frac{1}{s-1} \left(p_0^{1-s} \left(\sqrt{1+p_0^2} - 1 \right) + \frac{1}{2} B_{\frac{1}{1+p_0^2}} \left(\frac{s-2}{2}, \frac{3-s}{2} \right) \right) \quad (8)$$

where $B_x(a, b)$ denotes the incomplete Beta-function, and $s > 2$ is assumed.

4 INTERACTION BETWEEN COSMIC RAYS AND MATTER

4.1 Coulomb losses

Here we are interested in the problem of the energy loss of cosmic rays in the interstellar and intergalactic gas. The basis of all electromagnetic interactions is the Coulomb scattering between electric charges, which allows for transfer of kinetic energy as the proton moves through a free electron gas. According to Gould (1972), the total energy loss of a proton by Coulomb losses in a plasma is given by:

$$-\left(\frac{dT_p(p)}{dt} \right)_c = \frac{4\pi e^4 n_e}{m_e \beta c} \left[\ln \left(\frac{2m_e c^2 \beta p}{\hbar \omega_{pl}} \right) - \frac{\beta^2}{2} \right]. \quad (9)$$

Here, $\omega_{pl} = \sqrt{4\pi e^2 n_e / m_e}$ is the plasma frequency and n_e is the number density of free electrons. The result is independent of the mass m_p of the incident proton as long as the recoil of the proton can be neglected, i.e. $\gamma m_e c \ll m_p c$, with $\gamma = 1/\sqrt{1-\beta^2}$. Thus equation (9) is valid for $\gamma \ll m_p/m_e$. In a partially ionized medium the total loss of kinetic energy can simply be calculated by adding the losses due to excitation or ionization to the Coulomb losses as calculated here (Gould 1972).

4.2 Ionisation losses

Ionization energy losses are important for all charged particles, and for particles other than electrons and positrons they dominate over radiation energy losses at all but the highest energies. These ionization losses are governed by the Bethe-Bloch equation

(Groom & Klein 2000), which for moderately relativistic charged particles assumes the form:

$$\begin{aligned} -\left(\frac{dT_p(p)}{dt} \right)_I &= \frac{4\pi e^4}{m_e \beta c} \sum_Z Z n_Z L_0 \\ &= \frac{4\pi e^4}{m_e \beta c} \sum_Z Z n_Z \left[\ln \left(\frac{2m_e c^2 p^2}{I_Z b(\gamma)} \right) - \beta^2 - \frac{\delta_Z}{2} \right] \end{aligned} \quad (10)$$

where n_Z is the number density of atomic species with electron number Z , I_Z is the ionization potential, and L_0 is called the stopping number (Ziegler 1999). The quantity $b(\gamma) = \sqrt{1 + 2\gamma m_e / m_p + (m_e / m_p)^2}$ is a correction factor that accounts for the maximum kinetic energy that can be imparted to a free electron in a single collision (Groom & Klein 2000).

The density correction factor δ_Z accounts for the screening effect of a medium which becomes polarized as highly relativistic particles move through it (Martin & Shaw 2003). In this case the electromagnetic field of the ions may not be at the assumed free-space value, but is reduced by the dielectric constant of the medium (Ziegler 1999). The density correction factor δ_Z is usually negligible for gases (Groom & Klein 2000), but is given here for completeness:

$$\delta_Z = \begin{cases} 2y - D_Z & : (y_{1,Z} < y) \\ 2y - D_Z + a_Z (y_{1,Z} - y) / \ln 10^{k_Z} & : (y_{0,Z} < y < y_{1,Z}) \\ 0 & : (y < y_{0,Z}) \end{cases}$$

Here, $y = \ln(p)$, $D_Z = 1 - 2 \ln(\hbar \omega_{pl} / I_Z)$ and $y_{0,Z}$, $y_{1,Z}$, a_Z , k_Z are empirical constants which characterize the atomic species (Sternheimer 1952) and are given in table 1 together with the values for the ionization potentials I_Z of molecular hydrogen and helium. All hydrogen measurements were done with molecular hydrogen, but not much difference is expected when these values are adopted for atomic hydrogen.

As already pointed out earlier, the energy range of cosmic ray protons most important for the primordial chemistry is of order keV. The Bethe-Bloch equation in the form (10) is not valid at these low energies, and a correction term must be added to the square brackets of equation (10). The so called Bloch correction is important for slow particles (Mannheim & Schlickeiser 1994), and for protons it can be written as:

$$L_{Bloch} = \frac{1}{2} \left(\Psi(1) - \text{Re} \Psi \left(1 + \frac{i\alpha}{\beta} \right) \right) \quad (12)$$

where $\Psi(x)$ is the digamma function, the logarithmic derivative of the gamma function, and $\alpha = 1/137$ is the fine structure constant (Ziegler 1999).

With this corrections the Bethe-Bloch equation can be used for particles with velocities greater than the characteristic velocity of the medium's electrons, which is the orbital velocity in the K-shell of the atom (Mannheim & Schlickeiser 1994). For atomic hydrogen the orbital velocity can be derived from the Bohr atomic model and yields:

$$\beta_{orbit} = \frac{e^2}{\hbar c} \approx 0.0073. \quad (13)$$

For protons with velocities larger than β_{orbit} the Bethe-Bloch equation is in excellent agreement with the experimental values (Mannheim & Schlickeiser 1994).

At even lower particle velocities Ginzburg and Syrovatskii provide a useful ionization loss rate for slow ions (Ginzburg & Syrovatskii 1964), which for protons can be written as:

Element	Z	I_Z [eV]	$y_{0,Z}$	$y_{1,Z}$	a_Z	k_Z
He	2	24.6	$2.0 \ln 10$	$3.0 \ln 10$	0.98	4.11
H ₂	1	13.6	$1.76 \ln 10$	$3.0 \ln 10$	0.34	5.01

Table 1. Atomic data of He and H₂ as given by Sternheimer (1952). The hydrogen measurements were done with molecular hydrogen, but no significant changes for atomic hydrogen are expected within the accuracy needed for our purpose (Enßlin et al. 2006).

$$-\left(\frac{dT_p(p)}{dt}\right)_I = 2.11 \times 10^{-2} \beta^2 \sum_Z n_Z Z \frac{\text{eV}}{s}. \quad (14)$$

For proton velocities lower than β_{orbit} this agrees well with the experimental data of Whaling (1958). Then the total ionization energy loss formula is given by:

$$-\left(\frac{dT_p(p)}{dt}\right)_I = \begin{cases} \frac{4\pi e^4}{m_e \beta c} \sum_Z Z n_Z [L_0 + L_{Bloch}] & : (\beta > \beta_{orbit}) \\ 2.11 \times 10^{-2} \beta^2 \sum_Z n_Z Z \frac{\text{eV}}{s} & : (\beta < \beta_{orbit}). \end{cases} \quad (15)$$

Note that the derivation of the cosmic ray energy losses due to ionization neglects the details of the atomic shell structure. In order to obtain accurate energy losses, the particle electron collisions should be considered with detailed treatment of each target electron's orbital bonding, and as the particle slows down, a shell correction term should be added to equation (10) (Ziegler 1999). All the atoms considered in this work though, on average will always be in the ground state and thus no detailed study of the atomic shell corrections is needed. The correction would be at most 6% in the energy range 1 – 100 MeV (Ziegler 1999). Therefore, shell correction can be safely neglected, and equation (15) describes adequately the ionization losses of cosmic ray particles.

4.3 Hadronic losses

The known cosmic ray spectrum extends over energies from a few hundred MeV to 3×10^{20} eV (Biermann & Sigl 2001). Such high relativistic energies allow cosmic ray protons to overcome the Coulomb barrier and interact hadronically with the nuclei of the ambient matter. The fundamental theory underlying high energy collisions of hadrons is generally referred to as Quantum Chromo Dynamics (QCD) (Stanev 2004). As QCD predicts the creation of massive particles in collisions between hadrons if the incident particle possesses enough kinetic energy (Peskin & Schroeder 1995), these interactions, especially pion creation, are an important energy loss mechanism for cosmic ray protons at high energies. The lightest known mesons are pions, with masses $m_{\pi^{\pm}} c^2 = 139.57$ MeV for charged pions and $m_{\pi^0} c^2 = 134.98$ MeV for neutral pions (Martin & Shaw 2003). For positive and neutral pion production the lightest final states which conserve baryon number and electric charge are created by the processes



and



yielding a threshold energy $E_{CR}^0 \approx 1.22$ GeV, with a corresponding momentum threshold $p_{th} m_p c^2 \approx 0.79$ GeV (Martin & Shaw 2003).

The neutron produced in reaction (16) will decay into a proton after a mean lifetime of 886 s, so we basically end up with pions and two protons. This assures that the cosmic ray proton number density is conserved in these reactions. In subsequent processes the pions will decay via the channels

$$\pi^{\pm} \rightarrow \mu^{\pm} + \nu_{\mu}/\bar{\nu}_{\mu} \rightarrow e^{\pm} + \nu_e/\bar{\nu}_e + \nu_{\mu}/\bar{\nu}_{\mu} \quad (18)$$

and

$$\pi^0 \rightarrow 2\gamma \quad (19)$$

with mean lifetimes for charged pions of 2.6×10^{-8} s and for neutral pions of 8.4×10^{-17} s (Martin & Shaw 2003). However, the subsequent decay products are not considered further in this work.

The average kinetic energy loss of cosmic ray protons due to pion production has been calculated by Mannheim & Schlickeiser (1994) and can be written in the form

$$-\left(\frac{dT_p(p)}{dt}\right)_{had} = 0.65 c n_{nuclei} \sigma_{pp} T_p \Theta(p - p_{th}), \quad (20)$$

where n_{nuclei} is the number density of the target nucleon in the medium and $\sigma_{pp} = 3 \times 10^{-26}$ cm² is the cross section for pion production in proton collisions.

5 COUPLING BETWEEN COSMIC RAY PROTONS AND PRIMORDIAL GAS CHEMISTRY

In this Section we describe the method used and the approximations adopted to couple cosmic ray protons to the chemical evolution of a primordial gas.

5.1 Ionization rates

As a cosmic ray proton travels through matter it leaves behind a trail of ions. In accelerator experiments it is possible to measure the mean energy needed to create one electron-ion pair W_Z along the track, which clearly depends on the target material (Bakker & Segrè 1951). According to Heitler (1954) this average energy loss is representative for the average primary ionization of the cosmic ray proton.

Both the fractional number of cases in which a collision with an atom results in ionization rather than excitation to a discrete level and the average energy transferred to the ionized electron, are almost independent of the incident energy of the cosmic ray proton (Mannheim & Schlickeiser 1994). With these empirical observations and equation (15), the primary ionization rate for the chemical elements can be calculated as:

$$\lambda_{CR}^{prim} = \frac{\dot{\epsilon}_I(p_{min})}{W_Z n_Z}, \quad (21)$$

where $\dot{\epsilon}_I(p_{min})$ is the change of ionization energy density per time given as:

$$\dot{\epsilon}_I(p_{min}) = \int_{p_{min}}^{\infty} \left| \left(\frac{dT_p(p)}{dt} \right)_I \right| n(p) dp. \quad (22)$$

Here p_{min} is defined by the minimum energy necessary to ionize the atomic species (in the case of atomic hydrogen it is 13.6 eV) and W_Z is the mean energy expended per ion pair created by a proton. The values of W_Z were measured by Bakker & Segrè (1951) and Weiss & Bernstein (1956) for several elements, and are given in table 2 for molecular hydrogen and helium. The hydrogen measurements were done with molecular hydrogen, but no significant changes for atomic hydrogen are expected within the accuracy required here.

When a cosmic ray proton ionizes an atom, energy is transferred to the ejected electron as kinetic energy. Some of this energy will go into further ionization or excitation of atoms, followed by radiation, while some of the energy will go directly into heating

the medium (Spitzer & Scott 1969). Therefore, this first generation electrons give rise to additional ionization and more free electrons as long as their kinetic energy is above the ionization threshold energy.

According to Spitzer & Scott (1969) all secondary and higher generation ionization can be accounted for multiplying the primary ionization rate (21) by a factor $\xi = 5/3$. This holds up to an ionization fraction of $f = n_e/n_H \approx 10^{-2}$, while for higher ionization fractions secondary electrons loose their energy to Coulomb interactions with the free electron gas rather than to ionization of additional atoms (Spitzer & Scott 1969). As cosmic rays can raise the ionization fraction considerably, especially for low density gases, one should be aware of the errors that are introduced by using a constant ξ . However, at this stage of research we are mainly interested in finding an overall effect and therefore we treat ξ as a parameter. Comparison of calculations with $\xi = 5/3$ and $\xi = 1$ showed that not much difference arises from the different treatment of secondary electrons in the cases studied here (Jasche 2006).

With all the above simplifications the total ionization rate, including primary and higher generation ionizations, can be written as:

$$\lambda_{CR}^{tot} = \xi \lambda_{CR}^{prim}. \quad (23)$$

5.2 Cosmic ray input on the chemical network

The most important reactions by which cosmic ray protons influence the primordial chemical network are the following:

- (i) $P_{CR} + H \rightarrow P_{CR} + H^+ + e^-$
- (ii) $P_{CR} + He \rightarrow P_{CR} + He^+ + e^-$
- (iii) $P_{CR} + D \rightarrow P_{CR} + D^+ + e^-$
- (iv) $P_{CR} + H_2 \rightarrow P_{CR} + H_2^+ + e^-$
- (v) $P_{CR} + H^- \rightarrow P_{CR} + H + e^-$

where the electron detachment reaction (v) turned out to be negligible (Jasche 2006).

All these reactions conserve the cosmic ray proton number density, and therefore no exchange of particles between cosmic rays and medium needs to be considered. The ionization rates for the reactions can be calculated with equation (23) and the data taken from tables 1 and 2. Unfortunately, no experimental data for deuterium targets is available, and therefore we use the same values as for hydrogen, which should be a safe assumption for the accuracy required in this work. As 97% of cosmic ray-H₂ impacts lead to the formation of H₂⁺ via reaction (iv) no other destruction mechanism for molecular hydrogen by cosmic ray protons will be considered here in agreement with the literature (Hartquist & Williams 1996). However, inclusion of additional cosmic ray-H₂ reactions lead to the formation of additional H₂. Such reactions and also the influence of cosmic rays on other molecules like HD will be discussed in detail in forthcoming publications.

Whenever there is helium present in the medium, it will not only be ionized by the cosmic ray protons, but will also emit a 21.23 eV photon, as the remaining electron relaxes to a new shell configuration (Spitzer & Scott 1969). In principle this photon is capable of ionizing further atomic hydrogen. But since we consider a very rarefied medium and the flux of these photons is assumed to be low, they are expected to contribute insignificantly to the overall ionization rate.

Element	Z	W_Z [eV]
He	2	40.3 ± 0.8
H ₂	1	36.3 ± 0.7

Table 2. Experimental values of W_Z for molecular hydrogen (Bakker & Segrè 1951) and helium (Weiss & Bernstein 1956).

5.3 Heating rates

Cosmic rays can be an efficient heat source especially for a low density gas, and therefore their heat input to the medium must be considered. When the cosmic ray proton ionizes an atom, it transfers a certain amount of kinetic energy to the electron, which is either used for further excitation and ionization of atoms, or is distributed by elastic collisions to other species of the medium. In the latter case the overall kinetic temperature is raised.

The effect of heating by cosmic ray ionization and secondary electrons is not well described in the literature. The papers that mention heating by cosmic ray ionization are not very detailed and show some discrepancies (e.g. Mannheim & Schlickeiser (1994); Spitzer & Scott (1969)). Here we will provide a reasonable upper limit to the heat input.

Let E_{ion}^Z be the ionization threshold energy of an atom of atomic charge Z (for hydrogen $E_{ion}^1 = 13.6$ eV). Then the mean kinetic energy E_{kin} imparted to the primary electron in a single collision can be calculated as

$$E_{kin} = (W_Z - E_{ion}^Z). \quad (24)$$

In subsequent collisions the primary electron will on average ionize $\xi - 1$ atoms and therefore loose the additional kinetic energy $(\xi - 1)E_{ion}^Z$. Thus every primary ionization by a cosmic ray particle finally yields a temperature gain equivalent to an energy $E_{heat} = (W_Z - \xi E_{ion}^Z)$. Hence we can write the heating rate for cosmic ray ionization as

$$\Gamma_{CR}^{ion} = (W_Z - \xi E_{ion}^Z) \lambda_{CR}^{prim} n_Z = \left(\frac{W_Z}{\xi} - E_{ion}^Z \right) \lambda_{CR}^{tot} n_Z \quad (25)$$

which, for $\xi = 5/3$, means a heat input of $E_{heat} \approx 8.18$ eV for every ionization of hydrogen in a neutral medium. This heat input is an overestimation as the electron could have also lost energy to excitation which was not accounted for here. Thus, in a neutral medium less than 1/4 of the energy transferred from the cosmic ray proton is finally deposited as heat. Again, it should be noted that ξ decreases with increasing ionization fraction f and thus the heat input by cosmic rays will increase with f . As soon as a large fraction of the medium is ionized, the cosmic ray proton loses kinetic energy mainly due to Coulomb interactions with the free electrons of the medium, and all the kinetic energy imparted to the free electrons is equivalent to the heating energy E_{heat} .

The heating rate due to Coulomb interactions can be calculated by using equation (9):

$$\Gamma_{CR}^{coul} = \int_0^\infty \left(\frac{dT_p(p)}{dt} \right)_C n(p) dp. \quad (26)$$

The fact that the energy lost by cosmic ray protons in Coulomb interactions is directly transferred to heat of the medium is the reason why cosmic rays are an efficient heat source. Thus, once the gas is ionized to sufficiently high degrees the future fate of the medium will be defined by Coulomb heating solely.

6 METHOD

Here we will describe and discuss the numerical methods used to study the influence of early cosmic rays on primordial gas. In order to estimate the effects of cosmic ray protons on the chemistry of primordial gas, it is necessary to follow the chemical and thermal evolution of such gas along with the cosmic ray spectral evolution. Therefore we simulate a homogeneous and isotropic medium and follow the evolution of 13 species (H, H⁺, H⁻, H₂⁺, H₂, He, He⁺, He⁺⁺, HeH⁺, D, D⁺, HD and e⁻) self-consistently together with the spectral evolution of the cosmic ray protons. The code calculates the chemical evolution of primordial gas by taking into account 27 collisional rates (Appendix B), 17 radiative rates including CMB interactions (Appendix B) and 4 additional rates arising from the coupling of cosmic ray protons to the chemical network as mentioned earlier.

6.1 Code testing

The accuracy of the numerical scheme for the cosmic ray spectral evolution is checked by comparing the numerical results for the cosmic ray spectral evolution with the analytic equilibrium solution of equation (6) where we neglect the escape term. The deviation of the numerical results from the analytic ones is measured by

$$\delta n(p) = \frac{n_{\text{analytic}}(p) - n_{\text{numerical}}(p)}{n_{\text{analytic}}(p)}. \quad (27)$$

Here we do not consider any chemical evolution and assume a gas consisting of atomic hydrogen with a number density $n_{\text{H}} = 10^2 \text{ cm}^{-3}$. The cosmic ray spectrum is integrated from the lower boundary $p_{\text{min}} = 10^{-3}$ to the upper boundary $p_{\text{max}} = 10^3$ with a spectral index $s = 2.2$ and a cosmic ray energy density injection rate $\dot{\epsilon}_{\text{CR}} = 10^{-26} \text{ erg cm}^{-3} \text{ sec}^{-1}$.

The asymptotic steady state solutions are then compared for two scenarios. In the first scenario we consider that the cosmic rays interact with a totally neutral medium, while in the second we choose a totally ionized gas. The results are plotted in figure 1. The numerical solutions are nearly identical to the analytic ones. At the highest momenta the boundary effects lead to some deviations, which are still within the accuracy needed for this work. In any case these will not affect the calculations considered here since those high momenta are far beyond the region of interest for cosmic ray ionization. Therefore the calculations done in this work will not suffer from accuracy losses due to numerical effects.

Testing the chemical network is more difficult as no analytic solution exists. For this reason, we have chosen to check the behavior of the code against results present in the literature. We run a simulation to follow the chemical evolution of the intergalactic medium from redshift 10^4 to 0 and compare the results with those of Galli & Palla (1998).

For our calculations we adopt a Λ CDM cosmological model with $\Omega_{\Lambda} = 0.73$, $\Omega_m = 0.27$ and $H_0 = 71 \text{ km sec}^{-1} \text{ Mpc}^{-1}$. As initial conditions we assume a completely ionized gas with mass fractions $f_{\text{H}} = 0.76$, $f_{\text{He}} = 0.24$ and $f_{\text{D}} = 1.8 \times 10^{-5} f_{\text{H}}$, as predicted by nucleosynthesis (Smith et al. 1993). The result is presented in figure 2. From a comparison between the results obtained in this work and those of Galli and Palla, it is clear that the main features of the chemical evolution are very well reproduced by the code, although some minor differences are present. These arise because of the slightly different sets of chemical rates used and because Galli and Palla included more chemical species.

Finally as chemical reactions conserve the mass of the system we checked that the mass remains constant throughout the calculations.

6.2 The simulation

The gas in the simulations consists of the primordial elements H, D and He with the mass fractions $f_{\text{H}} = 0.76$, $f_{\text{He}} = 0.24$ and $f_{\text{D}} = 1.8 \times 10^{-5} f_{\text{H}}$ (Smith et al. 1993).

The parameters that determine the cosmic ray spectral evolution are set as follows. We set the boundaries for the integration region in momentum space at $p_{\text{min}} = 10^{-3}$ and $p_{\text{max}} = 10^4$, and assume the momentum cutoff p_0 in equation (7) to coincide with p_{min} . The spectral index s of the injected power-law spectrum is assumed to be $s = 2.2$, as expected for Fermi-acceleration at shocks (Mannheim & Schlickeiser 1994). This gives $\kappa(s, p_{\text{min}}) = 4.95$. The upper boundary p_{max} is much higher than the range of momentum expected to be important for the chemical network, and therefore boundary effects arising from the numerical integration of the cosmic ray spectrum will not interfere with the calculations of the chemical network. In order to restrict the number of parameters, the escape of cosmic ray particles from the medium under consideration is assumed to be negligible and therefore their escape time is set to $\tau = \infty$. This implies that either the gas occupies an infinite volume, or magnetic fields capable of confining the cosmic rays in the region of interest are present. As already discussed in Section 5.1 in the following we will usually adopt $\xi = 5/3$ and a mean heat input per ionization of $E_{\text{heat}} = 8.18 \text{ eV}$ for hydrogen and 4.0 eV for helium.

As not much about primordial cosmic ray sources and the regions in which cosmic rays might be present in the early universe is known, the code was used to run a large number of simulations in order to explore a wide range of the $\dot{\epsilon}_{\text{CR}} \times n$ parameter space.

Tests with an additional UV photon background field, as it might arise from the very first stars, showed that in the presence of ionizing photons the influence of cosmic rays is usually subdominant. We therefore consider only regions that are shielded from ionizing photon radiation, but the treatment of H₂ dissociating photons with energies in the range of the Lyman and Werner transitions (11.2-13.6 eV) is included (Thielens 2005). As only this small range of photon energy is of interest, we may assume a constant photon flux F . In the following we will refer to these dissociating photons as soft ultraviolet (SUV) radiation. No radiative transfer of photons is considered in this work, and therefore the dissociating background flux must be understood as a mean flux of photons in the gas. In reality, the molecules in the outer regions of the gas cloud absorb some of the dissociating photons resulting in a decrease of the dissociating radiation toward the inner regions (Thielens 2005). This self-shielding mechanism is clearly dependent on the gas density and distribution and therefore the mean flux of photons in the medium will in general depend on the total number density n and the sources that produce it.

7 RESULTS

In this Section we will discuss the effects of CR protons on the chemistry of a primordial gas as derived by our simulations.

It should be noted that cosmic rays are not able to destroy an initially available population of molecular hydrogen. As the electron detachment from H⁻ by cosmic rays is negligible the only possible destruction mechanism for molecular hydrogen is H₂ ioniza-

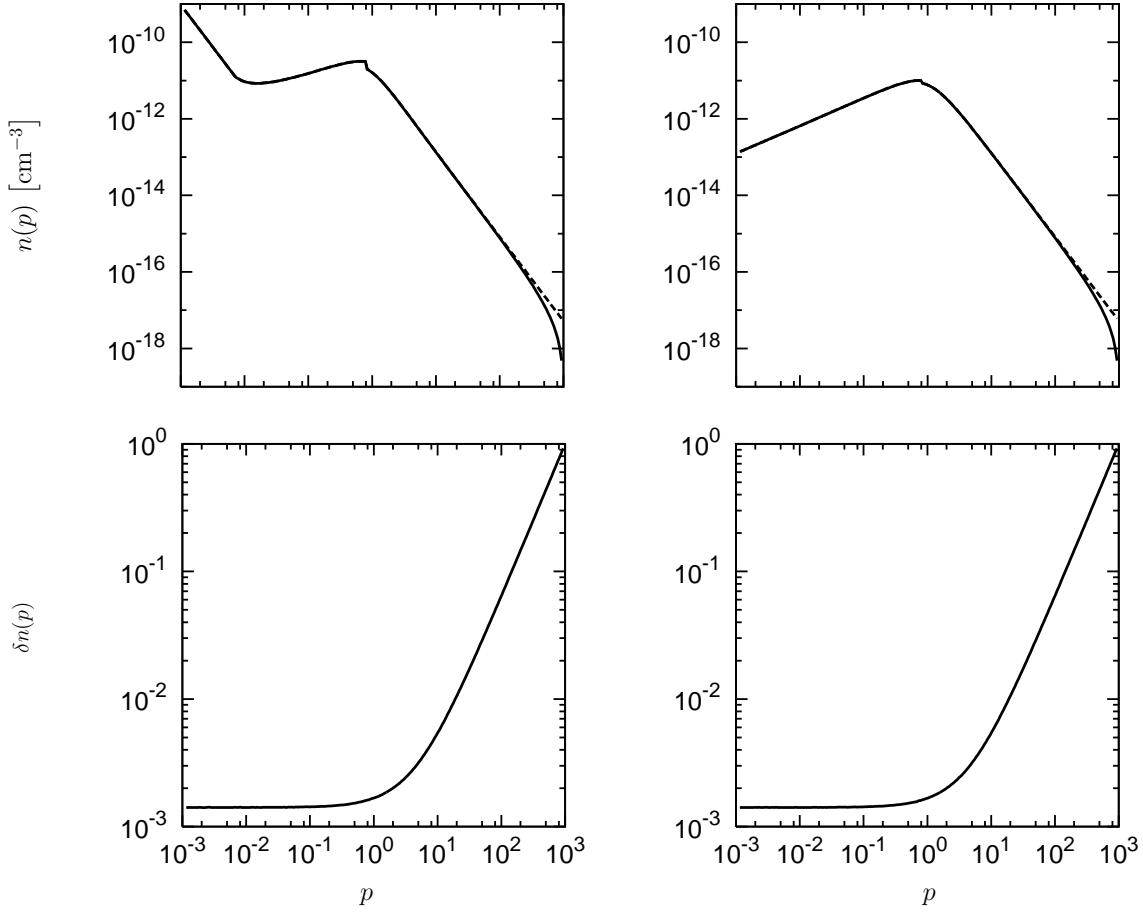


Figure 1. Upper panels: cosmic ray spectrum after interaction with a neutral (left panel) and an ionized (right panel) gas. The dashed (solid) lines indicate the analytic (numerical) results. Lower panels: $\delta n(p)$ for a neutral (left panel) and an ionized (right panel) gas.

tion. Nevertheless, as soon as cosmic rays are strong enough to sufficiently ionize molecular hydrogen, they also provide enough free electrons by ionizing the atomic species, resulting in a net production of H_2 (Jasche 2006). Therefore, cosmic rays do not interfere with any other chemical process that leads to the formation of molecular hydrogen. This suggests that the final abundance of H_2 can be written as:

$$n_{\text{H}_2} \approx n_{\text{H}_2}^0 + \Delta n_{\text{H}_2} \quad (28)$$

where $n_{\text{H}_2}^0$ is the initial number density of molecular hydrogen, and Δn_{H_2} is the number density produced by cosmic rays in a purely atomic gas of the same total number density.

The simple dependence of the overall behavior of n_{H_2} on its initial abundance allows to make some more general considerations. Let us assume to have a gas cloud with initial H_2 abundance $n_{\text{H}_2}^0 \geq 0$ in thermal and chemical equilibrium in the absence of cosmic rays. If H_2 line cooling is the main cooling mechanism, this implies that $\Gamma = \Lambda_{\text{H}_2}(n_{\text{H}_2}^0)$, where Γ includes all heating sources with exception of cosmic rays. When cosmic rays interact with the gas cloud, its temperature change can be written as:

$$\begin{aligned} \frac{3}{2} n k_B \Delta T &= \Gamma + \Gamma_{\text{CR}} - \Lambda_{\text{H}_2} \\ &= \Gamma + \Gamma_{\text{CR}} - [\Lambda_{\text{H}_2}(n_{\text{H}_2}^0) + \Lambda_{\text{H}_2}(\Delta n_{\text{H}_2})] \\ &= \Gamma_{\text{CR}} - \Lambda_{\text{H}_2}(\Delta n_{\text{H}_2}), \end{aligned} \quad (29)$$

if we assume that all additional heating sources remain constant and equal to the initial H_2 -cooling. Here we have used the fact that Λ_{H_2} in thermal and chemical equilibrium is proportional to the H_2 number density. This implies that the temperature change induced by the interaction of cosmic rays and a gas with any initial H_2 abundance can be estimated simply from the balance between Γ_{CR} and the H_2 cooling of an initially atomic gas. The advantage is that we can explore a wider physical condition range without knowing the exact initial abundance of H_2 and the details of heating sources other than cosmic rays.

Note that this separation of the chemical network into a purely atomic part, which is influenced by the cosmic rays, and an unchanged part with initial molecular hydrogen, must not be understood as a rule. This approximation is only valid under the assumptions presented here, and if the number density of atomic hydrogen does not change much.

Therefore, we will start our calculations from a neutral purely atomic gas of primordial composition, and all molecular hydrogen H_2 will be understood as the additionally produced molecular hydrogen Δn_{H_2} .

7.1 H_2 and temperature

The behavior of the chemical network under the radiation by cosmic ray protons is not well known. What we expect from the cou-

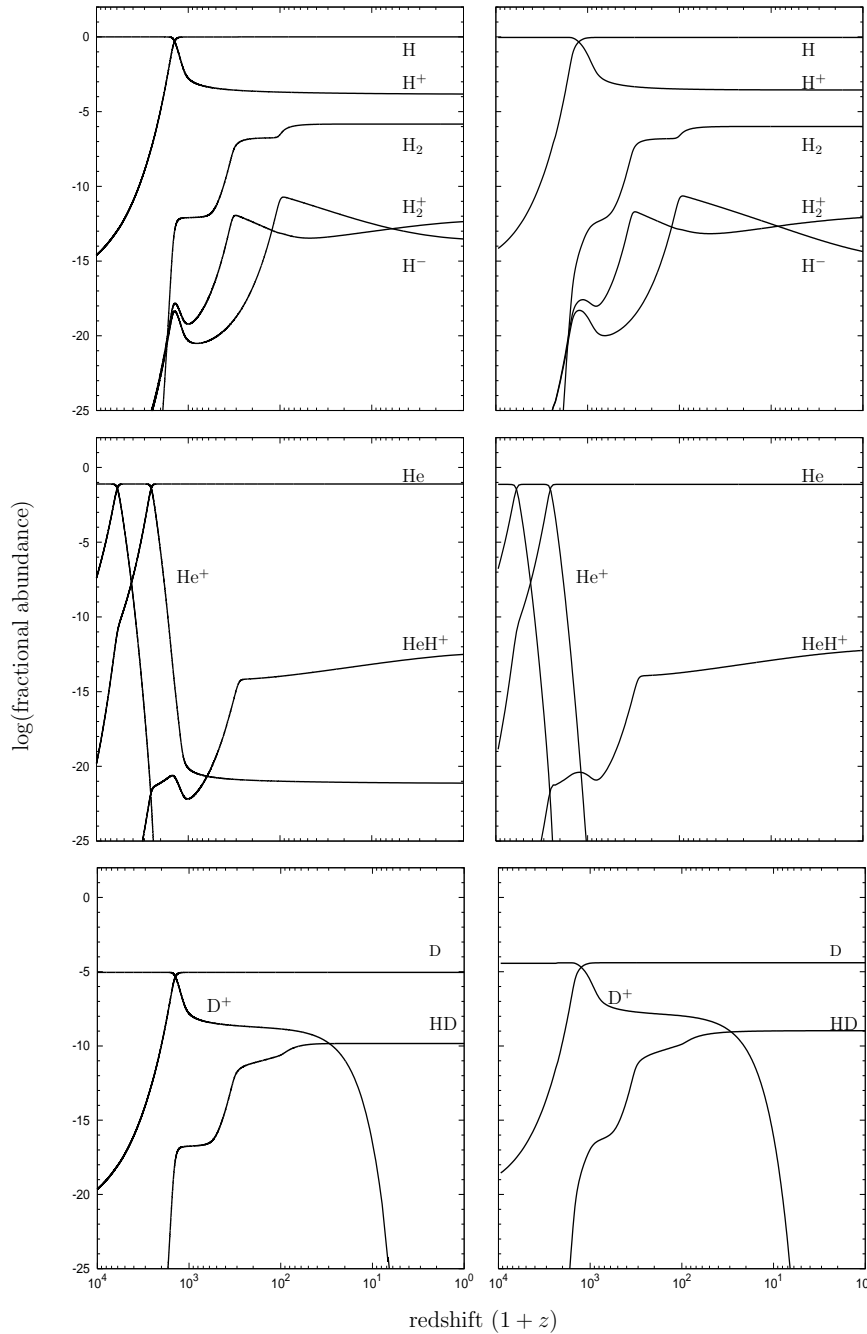


Figure 2. Chemical evolution of a primordial gas described in this work (left panels) and in Galli & Palla (1998) (right panels).

pling between the primordial chemical network and cosmic rays is an enhancement in the number density of H_2 , as cosmic rays ionize the atomic species and provide additional free electrons. This would eventually result in a net cooling of the gas by H_2 line emission if:

- (i) H_2 is produced on sufficiently short timescales and H_2 line cooling always outweighs cosmic ray heating;
- (ii) the gas is ionized only moderately to provide sufficient atomic hydrogen allowing for high H_2 formation rates.

The line cooling function Λ_{H_2} of molecular hydrogen depends on the gas temperature T . As in a low temperature gas the colliding

particles on average do not possess enough kinetic energy to excite the rotational modes of molecular hydrogen, cooling by H_2 line emissions becomes more and more inefficient at lower temperatures. Therefore we expect a minimum temperature at which no further cooling by molecular hydrogen is possible and cooling is balanced by the heating of cosmic rays.

As Λ_{H_2} depends on n_{H_2} , sufficient amounts of molecular hydrogen must be produced on short timescales to radiate away the heat input to the medium. For the formation of H_2 , free electrons and atomic hydrogen are needed. As cosmic rays ionize the medium they produce additional free electrons, but at the same time reduce the number of neutral hydrogen atoms. Therefore we expect

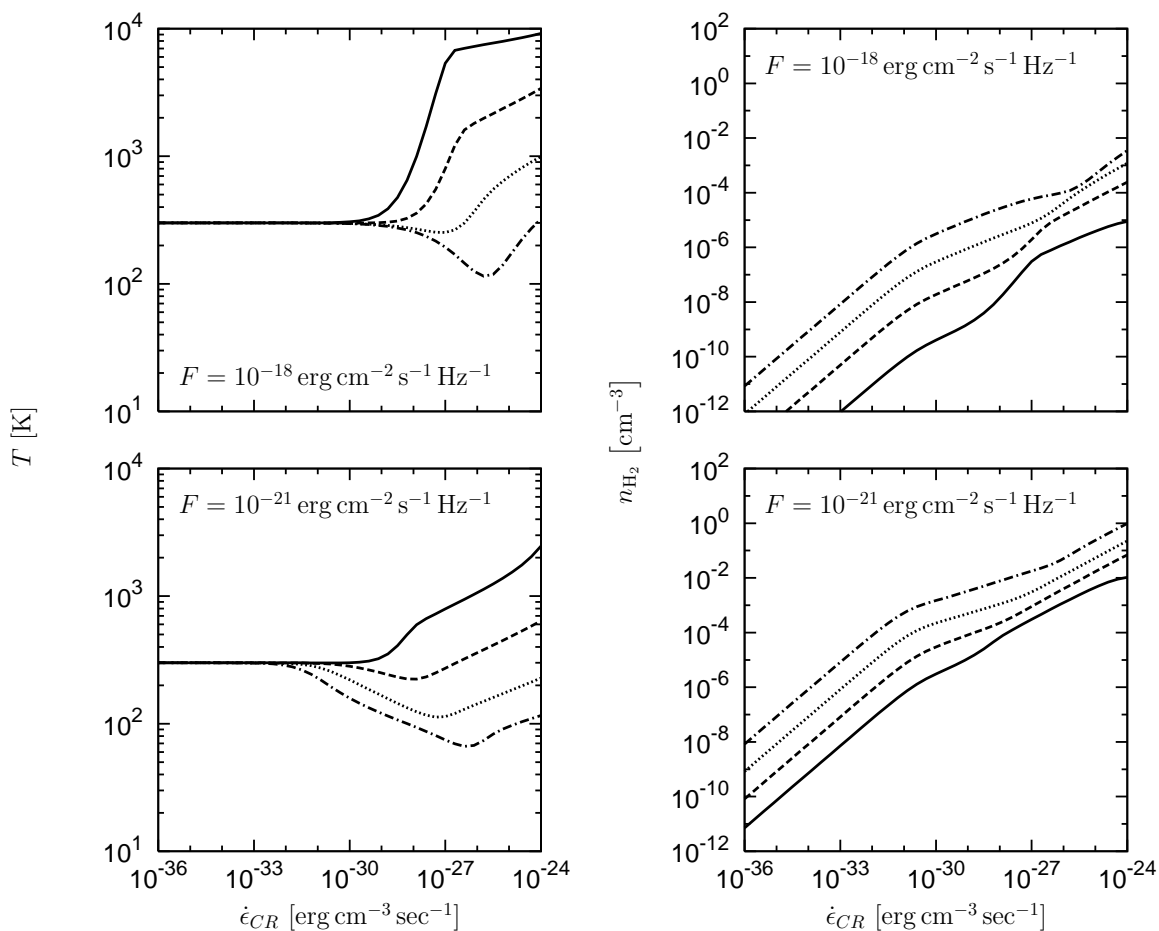


Figure 3. The left panel shows the final temperature and the right panel displays the final H_2 number density as a function of $\dot{\epsilon}_{CR}$ for two different SUV background fluxes. Different curves refer to different total number densities: $n = 1$ (solid line), 10 (dashed line), 100 (dotted line) and 1000 cm^{-3} (dash-dotted line). The initial temperature is $T_0 = 300 \text{ K}$.

a lower H_2 formation rate once a considerable fraction of the atomic hydrogen is ionized.

To assess all these effects we run simulations with gas of four different total number densities ($1\text{--}1000 \text{ cm}^{-3}$) and cosmic ray energy injection rates $\dot{\epsilon}_{CR}$ ranging from 10^{-36} to $10^{-24} \text{ erg cm}^{-3} \text{ s}^{-1}$, with different SUV background fluxes F . The evolution of the chemical network is followed over a time of 0.47 Gyr during which $\dot{\epsilon}_{CR}$ is assumed to be constant. After this integration time the gas has reached nearly thermal and chemical equilibrium, and not much change is observed beyond it.

The final values for the temperature T and the number density of molecular hydrogen n_{H_2} are plotted in figure 3 and figure 4 as a function of $\dot{\epsilon}_{CR}$ for simulations with initial temperature $T_0 = 300 \text{ K}$ and 3000 K respectively.

The overall observed effect is counterintuitive, as the gas cools with higher energy injection by cosmic rays. As can be seen in the plots, the temperature behavior (left panels) is highly dependent on the given environmental conditions, i.e. the total number density n , the initial gas temperature T_0 , the cosmic ray source strength $\dot{\epsilon}_{CR}$ and the SUV background flux. As expected from the previous discussions the final temperature is no monotonic function of the cosmic ray energy density injection rate $\dot{\epsilon}_{CR}$. Beyond a certain value of $\dot{\epsilon}_{CR}$, which also depends on the total gas number density n , cosmic rays start heating the gas again instead of inducing further cooling.

In addition we observe that gas with lower density is more likely to be heated by cosmic rays than gas of higher density, as here production of molecular hydrogen is easier and H_2 -line cooling is more efficient.

The data also show a considerable impact of the SUV background on the thermal evolution of the medium. A strong dissociating background suppresses the formation of molecular hydrogen and thus H_2 line cooling counterbalances the cosmic ray heating less efficiently. With a dissociating flux of $F = 10^{-18} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1}$ the production of molecular hydrogen is suppressed by a factor of 10^{-3} compared to the fiducial calculations with $F = 10^{-21} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1}$, resulting in effectively stronger heating by cosmic rays.

The choice of the initial temperature is critical for the evolution of the gas, as can be seen by a comparison between figure 3 and figure 4, which immediately shows that the effect of cosmic ray induced cooling is much more efficient at high initial temperatures. This is due to several effects, the most important being the increase of the H^- formation rate with temperature and the fact that H_2 -line cooling is more efficient at higher temperatures. Beside these effects the slight decrease of the recombination rates of the species H , D and He with temperature helps to increase the population of free electrons needed to catalyze the formation of H_2 .

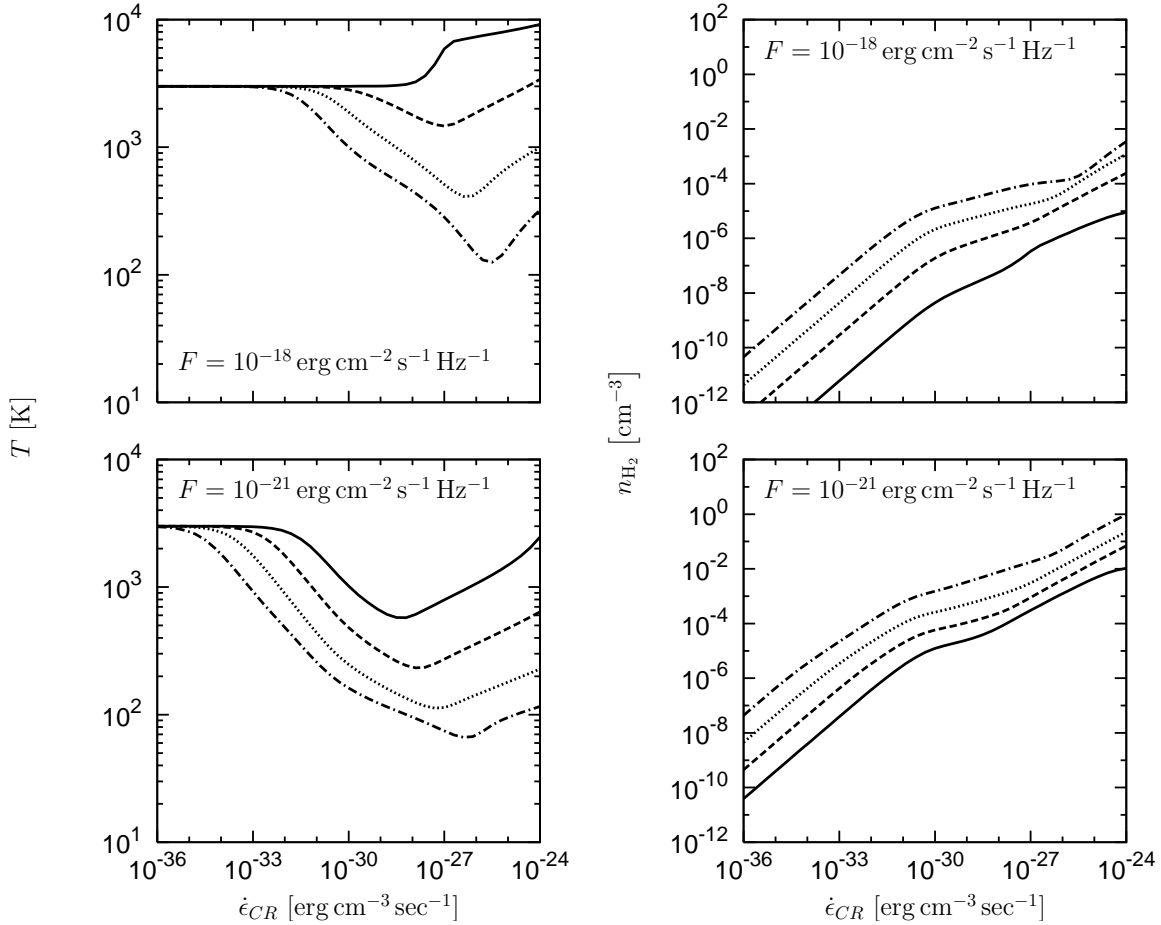


Figure 4. Same as figure 3 but for initial temperature $T_0 = 3000$ K.

It is interesting to note that with increasing initial temperature T_0 cosmic rays of lower intensity become more and more important. While, for example, for a gas with $T_0 = 300$ K and $n = 10 \text{ cm}^{-3}$ the first observable cooling effect begins at $\dot{\epsilon}_{CR} \sim 10^{-30} \text{ erg cm}^{-3} \text{ s}^{-1}$, the cooling effect starts already at $\dot{\epsilon}_{CR} \sim 10^{-33} \text{ erg cm}^{-3} \text{ s}^{-1}$ for the same gas simulated with $T_0 = 3000$ K. This suggests that in the latter case cooling induced by cosmic rays might be efficient also at number densities $< 1 \text{ cm}^{-3}$.

A closer comparison of figure 3 and figure 4 reveals another interesting feature. At the lowest energy injection rates the production of molecular hydrogen in gas $T_0 = 3000$ K is increased by nearly one order of magnitude compared to the calculations with gas starting from $T_0 = 300$ K. In contrast, at the highest simulated values of $\dot{\epsilon}_{CR}$ the results for temperature T and n_{H_2} are identical for both initial temperatures. In particular the results of calculations with these two initial temperatures are identical for values of $\dot{\epsilon}_{CR}$ higher than the energy injection rate at the minima in the temperature curves. Therefore beyond this point the chemical and thermal evolution of the gas does not depend on the initial conditions any more and all gas starting from whatever initial condition is converted to the same final state. Thus the minimum in the temperature curve defines a characteristic point for each gas.

7.2 Time evolution of parameter space

So far we have discussed the behavior of primordial gas under the influence of cosmic rays comparing only the final results of several calculations. It is instructive to study also the temporal evolution of the gas. Therefore, we display the evolution of the $\dot{\epsilon}_{CR} \times n$ -plane in time as a sequence of images. To have a satisfactory resolution of the parameter space we have run calculations for 40 different values of n , in the range $1-10^4 \text{ cm}^{-3}$, and of $\dot{\epsilon}_{CR}$ in the range $10^{-36}-10^{-24} \text{ erg cm}^{-3} \text{ s}^{-1}$. Each image of the $\dot{\epsilon}_{CR} \times n$ -plane then consists of 1600 points, where each point represents a different simulation.

In figure 5 we present some snapshots of a simulation with $T_0 = 2000$ K and $F = 10^{-21} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1}$. It can be seen that molecular hydrogen forms from the very beginning of the simulation, at times when no change in temperature can be observed yet. Initially we observe the highest effect in correspondence with high values of the energy density injection rate $\dot{\epsilon}_{CR}$ and total gas number density n , while the effect for low values of $\dot{\epsilon}_{CR}$ and n takes time to build up.

8 DISCUSSION

The calculations presented in this work give us a better understanding of the behavior of a primordial gas exposed to radiation of cosmic rays. In particular the parameter space maps, presented in fig-

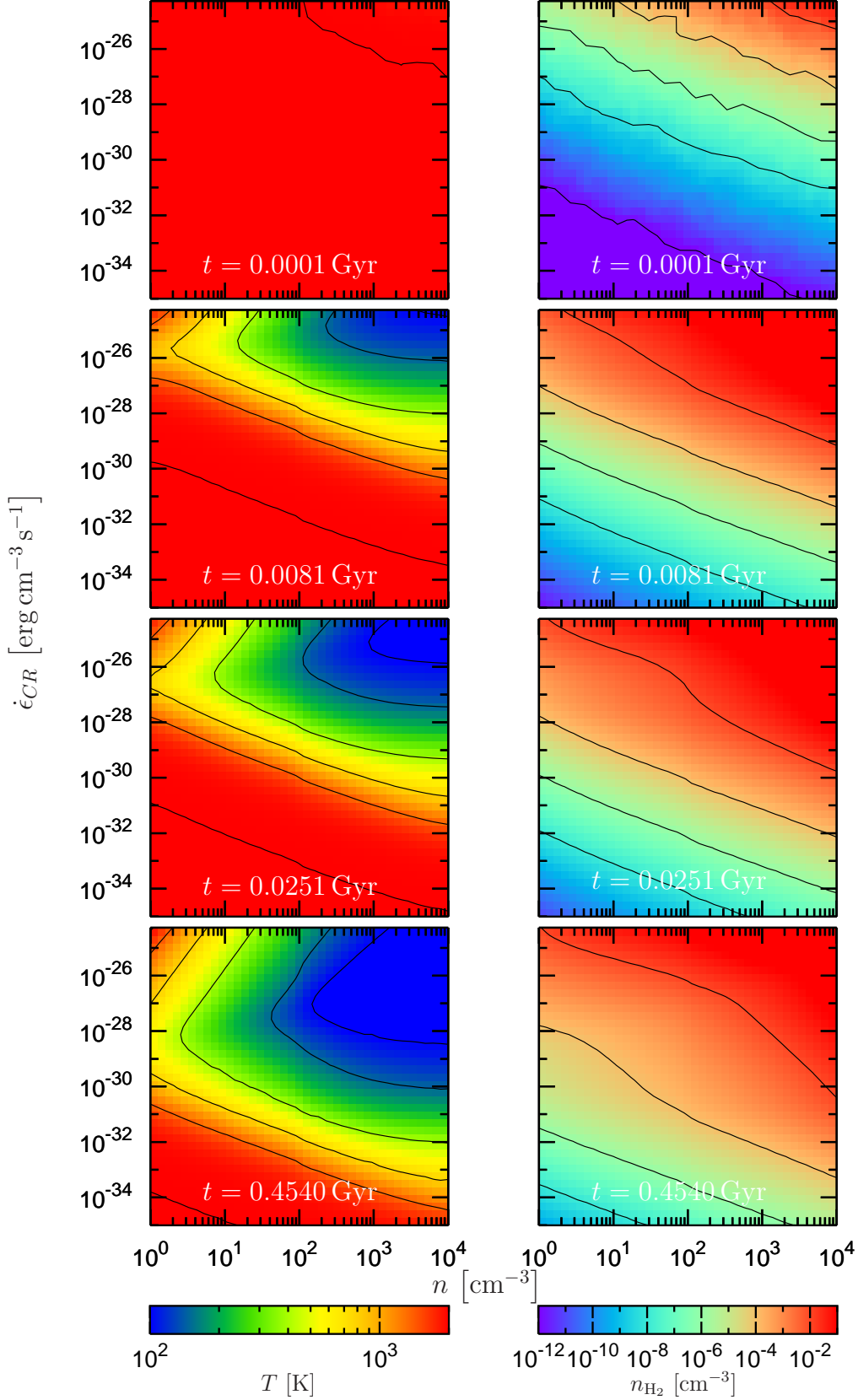


Figure 5. Time evolution of the $\dot{\epsilon}_{CR} \times n$ -plane for calculations with a neutral atomic gas at initial temperature $T_0 = 2000$ K, embedded in a dissociating flux with $F = 10^{-21} \text{ erg cm}^{-2} \text{ Hz}^{-1} \text{ s}^{-1}$. The panels refer to different times. The left panels display the temperature evolution while the right panels show the corresponding values for n_{H_2} . The superimposed contour plots join points of same temperature or same H_2 number density.

ure 5, can be used to identify regions of interest in the early universe. Here we want to discuss these results in more detail.

The most interesting conclusion that can be drawn from our calculations is that cosmic rays do not necessarily heat a gas, quite the contrary they might contribute to cooling. However, this trend is non-monotonic, as once the cosmic ray flux becomes larger than a critical value that depends on the gas initial conditions, heating dominates. This indicates that, to estimate the correct behavior of the thermal evolution of a primordial gas under the influence of cosmic rays, H_2 chemistry should be included self-consistently.

We studied the response of primordial gas to cosmic ray radiation in a variety of different environmental settings. In particular we were interested in the influence of the total gas number density n , the initial temperature T_0 , the SUV background and the cosmic ray intensity represented by $\dot{\epsilon}_{\text{CR}}$. We observed that the effect of cosmic rays depends strongly on the environment, especially on the initial temperature and the strength of the dissociating photon background. The results presented here therefore enable us to clearly define the environmental conditions for which this effect might be of interest. The following conditions are necessary for the cooling induced by cosmic rays to be efficient (although some cooling can be observed also for lower temperatures and densities):

- (i) A dissociating photon flux with $F < 10^{-18} \text{ erg cm}^{-2} \text{ Hz}^{-1} \text{ s}^{-1}$.
- (ii) Initial temperature of the gas $\sim 10^3 \text{ K}$.
- (iii) Total number densities of the gas $n \geq 1 \text{ cm}^{-3}$.
- (iv) Cosmic ray sources with $\dot{\epsilon}_{\text{CR}} > 10^{-33} \text{ erg cm}^{-3} \text{ s}^{-1}$.

We can therefore think of a variety of possible astrophysical scenarios in which cosmic rays might efficiently influence the chemistry of a primordial gas. For example, the first two conditions are in excellent agreement with the environment that can be found at the epoch of first structure formation, when objects with $T_{\text{vir}} \leq 10^4 \text{ K}$ collapse. As the cosmic microwave background is already much too weak to ionize, the only possible source for ionizing photon radiation would be stars that have not formed in sufficient amounts at these times. During the process of structure formation shock heated gas can contribute to the ultraviolet background by thermal emissions. However, these fluxes are expected to be small, especially for small structures, and in case of the SUV background do not exceed values of $F \sim 10^{-21} \text{ erg cm}^{-2} \text{ Hz}^{-1} \text{ s}^{-1}$ (Miniati et al. 2004). In addition, X-rays can contribute to ionization. These high energetic photons arise from free-free interactions of the electrons in the shock heated gas. As soft X-rays do not penetrate deeply into clouds and the flux of hard X-rays is small, the ionization is expected to be dominated by cosmic rays in the regimes considered in this work (Thielens 2005). It should be noted that, to have a proper estimate of the relative importance of different ionization sources, a self-consistent calculation should be done. A more thorough study on effects of CR on early structure formation is deferred to future work.

The main goal of the calculations presented above was to get a better understanding of the cosmic ray chemistry and effects which affect the H_2 formation. Therefore in all calculations no volume evolution was considered. This introduces some systematic errors when we want to apply the results to real cosmological situations. As the gas expands or contracts when it is heated or cooled, the total number density of the gas particles changes as a response to temperature change. Therefore, when the gas starts to cool, its number density increases leading to a higher formation rate of H_2 . This effect might increase the overall H_2 formation rate for a gas which experiences cooling induced by cosmic rays. To properly assess the impact of the volume evolution on our calculations, a detailed

treatment of the gas collapse and the effects of cosmic ray pressure should be included. This is beyond the scope of this study and we defer a more thorough investigation to future work.

The conclusions drawn in this paper rely on the presence of CR protons in the early universe, but our knowledge about primordial CR is very limited. As already mentioned in the Introduction some possible sources of primordial CR are decaying primordial black holes, structure formation shocks or the very first Supernovae. There is also the possibility that weakly interacting massive particles (WIMPs) decay into protons and anti-protons (Diehl et al. 1995). This would be an interesting source for cosmic ray protons as it is homogeneously distributed in space. Unfortunately the proton and antiproton fluxes arising from the decaying WIMPs are expected to be too low to have any interesting impact on the gas cooling (Diehl et al. 1995).

A more promising cosmic ray source in the absence of stars may be structure formation shocks. Cosmological shock waves form abundantly in the course of structure formation, both due to infalling pristine cosmic gas, which accretes onto filaments, sheets and halos, as well as due to supersonic flows associated with merging structures (Pfrommer et al. 2006). These shocks are able to dissipate gravitational energy associated with hierarchical clustering into thermal energy of the gas contained in dark matter halos. Beside this, shocks are able to accelerate ions of the high energy tail of the Maxwellian velocity distribution of a thermal medium by diffusive shock acceleration (Pfrommer et al. 2006). This acceleration process produces a cosmic ray population with a power-law distribution of the particle momenta. For this reason structure formation shocks seem to be plausible cosmic ray sources. As in addition we do not expect strong UV fluxes during early structure formation (Miniati et al. 2004) our calculations could be applied to such a configuration. Numerical studies suggest that the mean energy density injection rate of cosmic rays from structure formation shocks at $z = 10$ is $\dot{\epsilon}_{\text{CR}} \approx 10^{-33} \text{ erg cm}^{-3} \text{ s}^{-1}$, where this value is averaged over a co-moving volume of $\approx (143 \text{ Mpc})^3$ (Pfrommer et al. 2006). Thus, the local value of $\dot{\epsilon}_{\text{CR}}$ might be much higher.

Once the very first stars appear, much more powerful cosmic ray sources become available. These early massive stars ($M \sim 100 M_{\odot}$) form from metal-free gas through molecular hydrogen cooling (Abel et al. 2002) and are likely to end either as supernova or a black hole (Wise & Abel 2005). Supernovae are believed to be very efficient particle accelerator (Biermann & Sigl 2001) and therefore could easily increase the abundance of an early cosmic ray population. This could help to make the effect observed in our calculations more efficient and trigger the formation of second generation stars. Unfortunately primordial stars produce a lot of UV radiation which might severely hamper the production of molecular hydrogen (Wise & Abel 2005). Also, as already pointed out earlier, in the presence of ionizing photons the effect of cosmic ray ionization is usually sub-dominant, and if the medium is partly ionized cosmic rays will rather heat by Coulomb heating than induce H_2 -line cooling. One should also note that stars produce metals which are far more efficient coolants than molecular hydrogen. Therefore, in order to observe the effects described in this work, cosmic rays have to extend further into space than the pollution by metals. For these reasons we do not expect any significant effect of cosmic ray induced cooling in the vicinity of the sites of the very first stars and supernovae.

If, however, cosmic rays would be able to travel further away than the ionization front and the metal polluted area built up by the progenitor, they might contribute to the formation of molecular hydrogen in the ambient neutral medium. Anyway, such a scenario

would require detailed knowledge about the propagation properties of cosmic rays and magnetic fields in the early universe, which we presently do not have.

9 CONCLUSION

In this work we studied the influence of an early cosmic ray population on the chemistry of primordial gas. We developed a computer code to couple self-consistently the chemistry of a gas of primordial composition with the spectral evolution of cosmic rays permeating this medium. The code was then used to study the response of the gas in a variety of environmental settings. The main results of these calculations can be summarized as follows:

- (i) Cosmic rays do not necessarily heat, quite the contrary they can contribute efficiently to the cooling of a medium.
- (ii) Cosmic rays influence the chemical state of a gas appreciably. In particular they catalyze the formation of molecular hydrogen.
- (iii) The impact of cosmic rays on the gas chemistry depends highly on the environmental conditions.

However, the detailed processes of cosmic ray production and propagation in the early universe are yet unclear and further investigation will be needed to completely understand a potential relevance of cosmic rays for early structure formation.

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Cooling rate	Reference
$\Lambda_{line}(H)$	Cen (1992a) and Black (1981)
$\Lambda_{line}(He)$	Cen (1992a) and Black (1981)
$\Lambda_{line}(He^+)$	Cen (1992a) and Black (1981)
$\Lambda_{ion}(H)$	Cen (1992a) and Shapiro & Kang (1987)
$\Lambda_{ion}(He)$	Cen (1992a) and Shapiro & Kang (1987)
$\Lambda_{ion}(He^+)$	Cen (1992a) and Shapiro & Kang (1987)
$\Lambda_{ion}(He)$	Cen (1992a) and Shapiro & Kang (1987)
$\Lambda_{rec}(H^+)$	Black (1981) and Spitzer (1978)
$\Lambda_{rec}(He^+)$	Black (1981) and Spitzer (1978)
$\Lambda_{rec}^{de}(He^+)$	Black (1981) and Spitzer (1978)
$\Lambda_{rec}(He^{++})$	Black (1981) and Spitzer (1978)
Λ_{Brems}	Black (1981)
$\Lambda_{compton}$	Peebles (1971)
Λ_{H^-diss}	Shapiro & Kang (1987)
$\Lambda_{H_2\text{ formation}}$	Abel et al. (1997)
$\Lambda_{H_2\text{ diss}}$	Shapiro & Kang (1987)
$\Lambda_{H_2\text{ line}}$	Galli & Palla (1998)

Table A1. Cooling rates and the corresponding references.

APPENDIX A: HEATING AND COOLING RATES

The cooling rates used in this work are given in table A1 together with the corresponding references.

The kinetic energy of particles (i.e. electrons) produced by photo-ionization and photo-dissociation will be the heat sources. According to Shapiro & Kang (1987) the heating rate due to these reactions is given by:

$$\Gamma = n_i \int_{\nu_{th}}^{\infty} (h\nu - h\nu_{th}^i) F(\nu) \sigma^i(\nu) \frac{d\nu}{h\nu}, \quad (A1)$$

where n_i and ν_{th}^i are the density and threshold energy of species i , respectively, $F(\nu)$ and $\sigma^i(\nu)$ are the radiation flux and the cross section for the reaction, respectively. Note that no radiative transfer is considered in equation A1.

APPENDIX B: CHEMICAL RATES

The chemical reactions implemented in our code are given in table B1 together with the references to the chemical rates.

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Reaction	Reference
$H + e^- \rightarrow H^+ + 2e^-$	Janev & Langer (1987)
$H^+ + e^- \rightarrow H + \gamma$	Abel et al. (1997)
$He + e^- \rightarrow He^+ + 2e^-$	Janev & Langer (1987)
$He^+ + e^- \rightarrow He + \gamma$	Cen (1992b) and Aldrovandi & Pequignot (1973)
$He^+ + e^- \rightarrow He^{++} + 2e^-$	AMDIS Database (1989) see Abel et al. (1997)
$He^{++} + e^- \rightarrow He^+ + \gamma$	scaling (e.g. see Osterbrock (1989))
$H + e^- \rightarrow H^- + \gamma$	Abel et al. (1997)
$H + H^- \rightarrow H_2 + e^-$	Abel et al. (1997), Shapiro & Kang (1987)
$H + H^+ \rightarrow H_2^+ + \gamma$	Shapiro & Kang (1987)
$H_2^+ + H \rightarrow H_2 + H^+$	Karpas et al. (1979)
$H_2 + H^+ \rightarrow H_2^+ + H$	Abel et al. (1997)
$H_2 + e^- \rightarrow 2H + e^-$	Donahue & Shull (1991)
$H_2 + H \rightarrow 3H$	Dove et al. (1986)
$H^- + e^- \rightarrow H + 2e^-$	Janev & Langer (1987)
$H^- + H \rightarrow 2H + e^-$	Abel et al. (1997)
$H^- + H^+ \rightarrow 2H$	Dalgarno & Lepp (1987)
$H^- + H^+ \rightarrow H_2^+ + e^-$	Abel et al. (1997)
$H_2^+ + e^- \rightarrow 2H$	Abel et al. (1997)
$H_2^+ + H^- \rightarrow H_2 + H$	Dalgarno & Lepp (1987)
$D^+ + e^- \rightarrow D + \gamma$	Galli & Palla (1998)
$D + H^+ \rightarrow D^+ + H$	Galli & Palla (1998)
$D^+ + H \rightarrow D + H^+$	Galli & Palla (1998)
$D^+ + H_2 \rightarrow HD + H^+$	Smith et al. (1982)
$HD + H^+ \rightarrow H_2 + D^+$	Smith et al. (1982)
$He + H^+ \rightarrow HeH^+ + \gamma$	Roberge & Dalgarno (1982)
$HeH^+ + H \rightarrow He + H_2^+$	Karpas et al. (1979)
$HeH^+ + e^- \rightarrow He + H$	Yousif & Mitchell (1989)
$H + \gamma \rightarrow H^+ + e^-$	Osterbrock (1974)
$He + \gamma \rightarrow He^+ + e^-$	Osterbrock (1974)
$He^+ + \gamma \rightarrow He^{++} + e^-$	Osterbrock (1974)
$H^- + \gamma \rightarrow H + e^-$	de Jong (1972)
$H_2 + \gamma \rightarrow H_2^+ + e^-$	Oneil & Reinhardt (1978)
$H_2^+ + \gamma \rightarrow H + H^+$	Osterbrock (1974)
$H_2^+ + \gamma \rightarrow 2H^+ + e^-$	Shapiro & Kang (1987)
$H_2 + \gamma \rightarrow H_2^+ \rightarrow H + H$	Abel et al. (1997)
$H_2 + \gamma \rightarrow H + H$	Abel et al. (1997)
$H + \gamma_{CMB} \rightarrow H^+ + e^-$	Galli & Palla (1998)
$He + \gamma_{CMB} \rightarrow He^+ + e^-$	Galli & Palla (1998)
$He^+ + \gamma_{CMB} \rightarrow He^{++} + e^-$	Galli & Palla (1998)
$H^- + \gamma_{CMB} \rightarrow H + e^-$	Galli & Palla (1998)
$H_2 + \gamma_{CMB} \rightarrow H_2^+ + e^-$	Galli & Palla (1998)
$H_2^+ + \gamma_{CMB} \rightarrow H + H^+$	Galli & Palla (1998)
$H_2^+ + \gamma_{CMB} \rightarrow 2H^+ + e^-$	Galli & Palla (1998)
$D + \gamma_{CMB} \rightarrow D^+ + e^-$	Galli & Palla (1998)
$HeH^+ + \gamma_{CMB} \rightarrow He + H^+$	Galli & Palla (1998)

Table B1. Reactions and references for the different chemical rates.