Radiative feedback and cosmic molecular gas: numerical method

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ABSTRACT

We present the results from self-consistent numerical simulations of cosmic structure formation with a multifrequency radiative transfer scheme and non-equilibrium molecular chemistry of 13 primordial species ($e^-$, H, H\textsuperscript{+}, H\textsuperscript{−}, He, He\textsuperscript{+}, He\textsuperscript{++}, H\textsubscript{2}, H\textsubscript{2}\textsuperscript{+}, D, D\textsuperscript{+}, HD and HeH\textsuperscript{+}), performed using the simulation code GADGET. We describe our implementation and we show tests for ionized sphere expansion in a static and dynamic density field around a central radiative source, and for cosmological abundance evolution coupled with the cosmic microwave background radiation. As a demonstrative application of radiative feedback on molecular gas, we also run cosmological simulations of early structure formation in a $\sim$1-Mpc sized box. Our tests agree well with analytical and numerical expectations. Consistent with other works, we find that ionization fronts from central sources can boost $H_2$ fractions in shock-compressed gas. The tight dependence on $H_2$ also leads to a corresponding boost of HD fractions. We see a strong lowering of the typical molecular abundances up to several orders of magnitude, which partially hinders further gas collapse of pristine neutral gas. This clearly suggests the need for reionized gas or metal cooling in the formation of the following generation of structures.

Key words: radiative transfer – methods: numerical – cosmology: theory.

1 INTRODUCTION

Our existing understanding of cosmic structure formation relies on observations of a Universe that is expanding at a rate of $H_0 \simeq 70$ km $s^{-1}$ Mpc$^{-1}$ and whose energy budget is largely dominated by a form of unknown dark energy or a cosmological constant, $\Lambda$, which contributes $\sim$70 per cent to the total cosmic energy content. The residual matter contribution is roughly $\sim$30 per cent, but only a very small fraction ($\sim$4 per cent) consists of ordinary baryonic matter, while the rest is unknown cold (i.e. non-relativistic) dark matter (DM). More precisely, recent determinations suggest $\Omega_{\text{m}} = 0.272$, $\Omega_{\Lambda} = 0.728$ and $\Omega_{\text{b}} = 0.044$ (Komatsu et al. 2011). In this framework, also called the $\Lambda$ cold dark matter ($\Lambda$CDM) model, cosmological structures can grow from the gravitational instability (Jeans 1902) of primordial matter fluctuations, which probably originated during the primordial inflationary epoch. These early perturbations represented the seeds that would develop into present-day galaxies and stars (Schwarzschild & Spitzer 1953) through gas cooling and condensation (Spitzer 1962). These can affect the surrounding environment through a number of mechanical, chemical and radiative processes, commonly known as feedback effects (on this topic, see the extensive review by Ciardi & Ferrara 2005).

Quantitatively speaking, linear perturbation analyses are usually performed to study the initial phases of gravitational collapse, where a Gaussian density distribution for the primordial matter fluctuations is assumed. The linear expansion of the continuity, Euler and energy equations can also be extended with higher-order corrections (e.g. Tseliakhovich & Hirata 2010; Greif et al. 2011; Maio, Koopmans & Ciardi 2011a; Stacy, Bromm & Loeb 2011) or non-Gaussian deviations (e.g. Grinstein & Wise 1986; Koyama, Soda & Taruya 1999; Komatsu et al. 2002; Grossi et al. 2007; Desjacques, Seljak & Iliev 2009; Maio 2011; Maio & Iannuzzi 2011; Maio & Khochfar 2012). However, in order to study non-linear regimes and feedback mechanisms, it is essential to perform numerical integrations and to use $N$-body/hydro simulations. Indeed, to capture early gas collapse, it is necessary to follow not only gravity and hydrodynamics, but also its full chemistry evolution and molecular formation. Because, in the cosmic medium, hydrogen (H) is the most abundant species with a cosmological mass fraction of $X_H \simeq 0.76$ (corresponding to $\sim$0.93 in number fraction), its contribution in gas cooling is likely to play a very relevant role, together with helium (He). However, although H and He collisional processes are able to cool the medium to $\sim$10$^4$ K via resonant line transitions, they are not capable of reducing the gas temperature further. At such low temperatures, thermal collisions are not able to excite the electrons to higher levels because of the large energy gaps (from a few to some tens of eV) of H and He atomic configurations. Saslaw & Zipoy (1967) proposed that gas cooling and fragmentation could...
be continued below \(\sim 10^4\) K by H\(_2\) cooling, down to \(\sim 10^2\)–\(10^3\) K. Later, Lepp & Shull (1984) suggested that the existence of primordial deuterium (D) could determine HD formation and consequent cooling, even below \(\sim 10^2\) K, down to several \(\sim 10\) K. During the last few decades, these problems have been tackled by collecting full reaction networks (Shapiro & Kang 1987; Puy et al. 1993; Abel et al. 1997; Hui & Gnedin 1997; Galli & Palla 1998; Uchida & Inutsuka 2000; Nakamura & Umemura 2002; Omukai et al. 2005; Glover & Abel 2008; Glover et al. 2010; Omukai, Hosokawa & Yoshida 2010) and by running high-resolution chemistry cosmological simulations, both in the standard CDM model (e.g. Abel, Bryan & Norman 2002; Bromm, Coppi & Larson 2002; Yoshida et al. 2003, 2007) and in dark-energy cosmological models (Maio et al. 2006). The effects of metal cooling have also been investigated in numerical simulations by joining molecular chemistry evolution with metal pollution and low-temperature fine structure transitions from, for example, C, O, Si and Fe (e.g. Maio et al. 2007). These studies clearly show the significance of metals in cosmological chemical evolution (chemical feedback) and they show how the rapidity of early enrichment from the first star formation episodes (see also Tornatore, Ferrara & Schneider 2007) has overcame gas molecular cooling (Maio et al. 2010, 2011b), marking the transition from the primordial, pristine star formation regime – the so-called Population III (popIII) regime – to the more standard Population II-I (popII-I) regime (Maio et al. 2010). This transition is often parametrized in terms of a minimum critical metallicity \(Z_{\text{crit}} \approx 10^{-4} Z_\odot\). However, given our ignorance about early dust production and low-temperature fine structure transitions from, for example, C, O, Si and Fe (e.g. Maio et al. 2007), we can indirectly use the chemical feedback, its effects on the dynamical and thermodynamical state of the cosmic gas, or its connections to the set-up of a turbulent medium dominated by hydro-instabilities (e.g. Maio et al. 2011a).

The first semi-analytical works (Haiman, Rees & Loeb 1997a,b; Haiman 1999) expected molecular hydrogen to be universally destroyed by ultraviolet (UV) stellar radiation in the LW band. Subsequently, one-dimensional, numerical studies of small- or intermediate-size boxes (\(\leq 1\) Mpc on a side), including RT coupled with hydrodynamics, have demonstrated that these predictions overestimated molecular destruction. Using a softened Lagrangian hydrodynamics particle–particle–particle–mesh (SLH-\(^3\)M) implementation, Ricotti, Gnedin & Shull (2001, 2002a, 2002b) have shown that, despite the stellar UV radiation, H\(_2\) can be rapidly reformed in the shock-compressed gas of the ionization fronts (I-fronts) of the H\(_{\text{II}}\) regions. This was the first suggestion of ‘positive’ feedback exerted by I-fronts on primordial structure formation.

Similar calculations, applied to individual haloes near to primordial stellar sources (e.g. Shapiro et al. 2004; Iliev et al. 2005; Hasegawa et al. 2009), have shown that UV radiation from popIII stars in crowded star-forming regions could photodissociate small (\(\sim 10^{-2} M_\odot\)) haloes in \(\gtrsim 100\) Myr. However, more recent studies (e.g. Susa & Umemura 2006; Susa et al. 2009; Hasegawa et al. 2009; Whalen et al. 2008; Whalen & Norman 2008; Whalen et al. 2010) have found that halo photoevaporation due to the first stars strongly depends on the features of the stellar sources and on the hydrodynamical properties of the collapsing cloud. Thus, it was found that radiative feedback can trigger gas cooling by catalysing H\(_2\) formation.

In order to overcome numerical issues in larger cosmological simulations (\(\gtrsim 1\) Mpc on a side), using a grid adaptive mesh refinement (AMR) implementation, Machacek, Bryan & Abel (2001, 2003) and Mesinger, Bryan & Haiman (2006, 2009), for example, adopted simple analytical prescriptions for a mean, uniform, UV background, assumed to be established after the early onset of star formation. In the way, detailed, AMR, popIII, star formation calculations in uniform LW backgrounds (O’Shea & Norman 2008; Wise & Abel 2008; Shang, Bryan & Haiman 2010) have confirmed that the LW background is much less destructive to new popIII stars than originally supposed; even by assuming extremely high background values of \(J \gtrsim 10^{-3} \text{erg cm}^{-2} \text{s}^{-1} \text{Hz}^{-1} \text{sr}^{-1} (\equiv J_{11})\), star formation is just delayed, not shut down.

In this essential review, we show briefly how the issues related to radiative feedback have been debated, and we highlight the numerous unknowns when dealing with RT and molecular chemistry. We aim to contribute to the scientific discussions and research that are already exist in the literature by implementing three-dimensional RT schemes, fully coupled with hydrodynamics, and non-equilibrium chemistry. At the end of the paper, together with chemistry and radiative transfer, we also consider additional feedback mechanisms that are relevant for cosmological structure formation (i.e. supernova feedback and wind feedback). This represents a step further with respect to previous implementations, because they usually focus on individual feedback processes. We perform the implementation within the widely used and well-tested numerical N-body/smoothed particle hydrodynamics (SPH) code \textsc{gadget} (Springel 2005), in its most recent and updated version. In this way, we can self-consistently study the effects of RT on chemical abundances, and we can pinpoint the basic consequences for the cosmological evolution of structures in the Universe. In Section 2, we describe the implementations of radiation (Section 2.1) and cosmic chemistry evolution (Section 2.2). In Section 3, we test our implementation by performing analyses of the Strömgren sphere problem (Section 3.1) – in
both a static (Section 3.1.1) and a dynamic (Section 3.1.2) density field – and chemical abundance evolution (Section 3.2). We then apply our method to cosmological structure formation simulations (Section 4). We summarize, discuss and conclude in Section 5.

2 IMPLEMENTATIONS

We use the parallel tree N-body/SPH code GADGET3, an extended version of the publicly available code GADGET2 (Springel 2005), and we modify it in order to couple chemistry evolution and RT. We give the details about the implementations of the RT (Section 2.1) and chemistry (Section 2.2) parts and, in Section 3, we give the results from our test runs.

2.1 Radiative transfer

To follow the propagation of radiation, we use the implementation of RT in GADGET3 (Petkova & Springel 2009) and we expand it to a multifrequency scheme. The original implementation is based on a moment method, where the closure relation is the optically thin variable Eddington tensor, suggested by Gnedin & Abel (2001). To follow the transport of radiation, we solve the equation of anisotropic diffusion for the photon number density per frequency \( n_\nu (\nu) \):

\[
\frac{\partial n_\nu (\nu)}{\partial t} = c \frac{\partial}{\partial x_j} \left( \frac{1}{k(\nu)} \frac{\partial n_\nu (\nu) h_j}{\partial x_i} \right) - c \kappa(\nu) n_\nu (\nu) + s_\nu (\nu).
\]  

(1)

Here, \( t \) is time, \( x_i \) and \( x_j \) are the coordinate components, \( c \) is the speed of light, \( \kappa(\nu) \) is the absorption coefficient, \( h_j \) are the components of the Eddington tensor, \( s_\nu (\nu) \) is the source function and the Einstein summation convention is adopted for all exponents \( i \) and \( j \).

The Eddington tensor is obtained by summing up the contributions from the sources of ionizing photons, and its components are given by

\[
h_{ij} = \frac{P_{ij}}{\text{Tr}(P_{ij})},
\]

(2)

where

\[
P_{ij}(x) = \int d^3 x' \rho_*(x') \frac{(x-x')_i(x-x')_j}{(x-x')^2} \]

(3)

is the radiation pressure tensor and \( \rho_* \) is the stellar density. The tensor is computed via a tree and it effectively removes the dependence of the scheme on the number of ionizing sources – an advantage in cosmological and galaxy formation simulations.

The source term is treated in a Strang-split fashion, where photons are first ‘injected’ into the medium surrounding the sources, and they are then ‘diffused’ via equation (1). Solving the equation for all particles in the simulation reduces this to a linear system of equations, which we solve implicitly by using a conjugate-gradient scheme, which ensures robustness and stability even for large time-steps.

For our multifrequency extension, we need to transform the photon number density to ionizing intensity, and vice versa. Because the photoionization rate in equations (7), which is discussed more in detail in Section 2.2, is obtained by integrating the intensity over frequency, we use a single photon number density in each frequency bin.

The photon number density per frequency is derived from the ionizing intensity, \( I(\nu) \), as

\[
n_\nu(\nu) = \frac{4\pi I(\nu)}{c h_\nu},
\]

(4)

where \( 4\pi \) is the full solid angle and \( h_\nu \) is the Planck constant. For any particle and at any time-step, the RT equation (1) is then solved for each frequency bin.

The intensity of the radiative source, \( I(\nu) \), depends on the particular problems treated. For stellar sources, a common, simple and suitable approximation (which we also adopt in the following) is a blackbody spectrum (see Fig. 1), with effective temperature dependent on the assumed stellar population. This treatment allows us to take into account contributions from a wide frequency range, even below the H-ionization energy of 13.6 eV. Indeed, as is evident from the plot in Fig. 1, the low-energy tail of the blackbody spectrum contributes to the LW band, and this will definitely affect the molecular evolution of the gas (see later).

We note that dealing with radiation below \( \sim 13.6 \) eV is a complicated problem that has been much debated (e.g. Haiman et al. 1997a,b; Omukai & Nishi 1999; Machacek et al. 2001; Kitayama et al. 2001; Ricotti et al. 2002a,b; Mackey, Bromm & Hernquist 2003; Dijkstra et al. 2004; Shapiro et al. 2004; Susa & Umemura 2004; Stacy et al. 2012), because of the many lines involved (76) in the LW band. Full, detailed modelling of RT in such regimes is beyond the aim of this paper and, at some levels, it might be superfluous (e.g. Ricotti et al. 2001), because the ionizing flux at high redshift \( (z) \) is dominated by radiation from neighbouring haloes (e.g. Ciardi, Ferrara & Abel 2000b), rather than from the soft-UV background in the LW band. Thus, \( \mathrm{H}_2 \) photodissociation is simply accounted for by using (e.g. Abel et al. 1997; Ricotti et al. 2001; Yoshida et al. 2003; Ahn & Shapiro 2007; Maiolino et al. 2007; Whalen & Norman 2008) the radiative rate obtained from integration of the source intensity over the LW range, 11.2–13.6 eV (see equation 7 in Section 2.2), shielded according to Draine & Bertoldi (1996).

2.2 Chemistry

To couple radiation with chemistry, we include non-equilibrium reactions for H, He and molecular evolution (whose ionization and dissociation energies are quoted in Table 1), by following a chemical network (see Table 2) of several species: \( \epsilon^+ \), H, \( \mathrm{He}^+ \), \( \mathrm{H}^+ \), \( \mathrm{He}^+ \), \( \mathrm{He}^{++} \), \( \mathrm{H}_2^+ \), \( \mathrm{D}^+ \), HD and HeH\(^+\). Besides some updates in the rates and in the reaction network, the implementation used is the same as the one in Maio et al. (2007, 2010) (and based on Abel et al. 1997; Galli & Palla 1998; Yoshida et al. 2003).

Figure 1. Intensity of a blackbody spectrum as a function of photon energy in eV for two different effective temperatures: \( 3 \times 10^5 \) K and \( 10^6 \) K. The vertical line marks the end of the LW band at 13.6 eV.
Table 1. Ionization energies in eV.

| Species | Ionization Energy |
|---------|------------------|
| H       | 13.6             |
| H⁻      | 0.7              |
| He      | 24.6             |
| He⁺     | 54.4             |
| D       | 14.9             |
| H₂      | 15.4             |
| HD      | 15.4             |
| HeH⁺    | 44.5             |

Table 2. Reaction network. Note that γ denotes photons.

| Reaction | References |
|----------|------------|
| H + e⁻ → H⁺ + e⁻ | A97/Y06/M07 |
| H⁺ + e⁻ → H + γ | A97/Y06/M07 |
| H + γ → H⁺ + e⁻ | A97/Y06/M07 |
| He + e⁻ → He⁺ + 2e⁻ | A97/Y06/M07 |
| He⁺ + e⁻ → He + γ | A97/Y06/M07 |
| He + γ → He⁺ + e⁻ | A97/Y06/M07 |
| He⁺ + e⁻ → He⁺⁺ + 2e⁻ | A97/Y06/M07 |
| He⁺⁺ + e⁻ → He⁺ + γ | A97/Y06/M07 |
| H + e⁻ → H⁺ + γ | GP98/Y06/M07 |
| H⁺ + γ → H + 2e⁻ | A97/Y06/M07 |
| H + H⁺ → H²⁺ + γ | GP98/Y06/M07 |
| H₂⁺ + γ → H + H⁺ | A97/Y06/M07 |
| H₂⁺ + γ → H + H²⁺ | A97/Y06/M07 |
| H\(^+\) + H₂ → H³⁺ | A97/M07 |
| H₂ + H → 2H + H | ST99/GB03/Y06/M07 |
| H⁺ + γ → H + 2e⁻ | A97/Y06/M07 |
| H⁺ + H⁺ → 2H + γ | GP98/Y06/M07 |
| H₂ + γ → H + H²⁺ | GP98/Y06/M07 |
| H₂ + H → H⁺ + H | GP98/Y06/M07 |
| H₂ + H₂ → 2H + H | ST99/GB03/Y06/M07 |
| H₂ + γ → H₂⁺ + e⁻ | A97/GP98/Y06/M07 |
| H₂ + γ → 2H + e⁻ | GP98/Y06/M07 |
| D + H₂ → HD + H | WS02/M07 |
| D²⁺ + H₂ → HD²⁺ + H⁺ | WS02/M07 |
| HD + H → D₂ + H₂ | SL98/M07 |
| HD + H⁺ → D²⁺ + H₂ | SL98/M07 |
| H⁺ + D + H → D²⁺ | SO2/M07 |
| H + D²⁺ → H⁺ + D⁺ | SO2/M07 |
| D²⁺ + e⁻ → D + γ | GP98 |
| D + γ → D²⁺ + e⁻ | GP98 |
| He + H⁺ → HeH⁺ + γ | RD82/GP98/M07 |
| HeH⁺ + H → He + H²⁺ | KA97/GP98/M07 |
| HeH⁺ + γ → He + H²⁺ | RD82/GP98/M07 |

* The references are as follows: P71, Peterson et al. (1971); KAH79, Karpas, Anichich & Huntress (1979); RD82, Roberge & Dalgallo (1982); SK87, Shapiro & Kang (1987); A97, Abel et al. (1997); GP98, Galli & Palla (1998); SL98, Stancil, Lepp & Dalgallo (1998); ST99, Shibib & Tennyson (1999); R01, Ricotti et al. (2001); WS02, Wang & Stancil (2002); SO2, Savin et al. (2002); GB03, Glover & Brand (2003); Y03, Yoshida et al. (2003); S04, Savin et al. (2004); Y06, Yoshida et al. (2007); M07, Maio et al. (2007). |

Because the main coolants at early times are H-derived molecules, H₂ (e.g. Slawas & Zipoy 1967) and HD (e.g. Lepp & Shull 1984), the inclusion of a large network is crucial to correctly resolve the hydrodynamics and the fragmentation processes of high-redshift gas, as also demonstrated by, for example, Abel et al. (1997), Yoshida et al. (2003, 2006), Maio et al. (2006, 2007, 2009, 2010, 2011a,b) and Maio & Iannuzzi (2011).

To take into account chemical evolution, at each time-step and for each species i, the time variation of its number density nᵢ is computed, for collisional and photoionization/photodissociation events, using

\[
\frac{dn_{\gamma,i}}{dt} = \sum_p \sum_q k_{pq,i} n_p n_q - \sum_i \kappa_i n_i n_i - k_{\gamma,i} n_i. \tag{5}
\]

Here, \(k_{\gamma,i}\) is the rate of creation of the species i from species p and q, \(\kappa_i\) is the destruction rate of the species i from collisions with species l and \(k_{\gamma,i}\) is the photoionization or photodissociation rate of species i as a result of radiation (see Table 1).

The collisional rates are given by

\[
k_{pq,i} = \int u \sigma_{pq,i}(u) f(u) du \tag{6}
\]

and analogous for \(k_{\gamma}\), where u is the relative velocity of particles p and q, \(\sigma_{pq,i}(u)\) is the interaction cross-section and \(f(u)\) is the Maxwellian velocity distribution function. More precisely, we do not compute the integrals on the fly, but instead we interpolate pre-computed tables (whose references are listed in Table 2) in order to speed up the code. These rates are temperature-dependent and they are expressed in units of number per volume per time (i.e. cm⁻³ s⁻¹) in the cgs system. As on the left-hand side, the first and second terms on the right-hand side of equation (5) have dimensions of a number density per unit time, cm⁻³ s⁻¹, in the cgs system.

As in Section 2.1, when the species i interacts with radiation \(\gamma\) (see Table 2) and becomes photoionized (as for H, D, H⁺, He and He⁺) or photodissociated (as for H₂, H₂⁺, HD and HeH⁺), the corresponding radiative rate \(k_{\gamma,i}\) can be written as

\[
k_{\gamma,i} = \int \frac{4\pi I(\nu)}{h\nu} \sigma_{\gamma,i}(\nu) d\nu = \int c \sigma_{\gamma,i}(\nu) n_i(\nu) d\nu. \tag{7}
\]

Here, 4πᵢ stands for isotropic radiation, \(I(\nu)\) is the source intensity as a function of frequency \(\nu\), \(\sigma_{\gamma,i}(\nu)\) is the cross-section for the given process, \(h\nu\) is the Planck constant, \(c\) is the speed of light and \(n_i(\nu)\) is the photon number density per frequency. In the final equality, we have made use of equation (4) in order to formally obtain the rate expression similar to equation (6). The radiative rates are probabilities per unit time, and they are given in s⁻¹ in the cgs system. So, the number of radiative interactions per unit time and volume between photons and particle i is \(k_{\gamma,i} n_i\). The latter quantity is added on the right-hand side of equation (5) when photon interactions are taken in consideration. As with the other terms in the equation, this is also given in units of number density per time (i.e. cm⁻³ s⁻¹) in the cgs system.

When talking about radiative interactions, we should consider that, while ionization energies (see Table 1) are uniquely defined, molecular dissociation energies might depend on the particular radiative process considered, and thus all the various channels must be taken into account. For example, LW radiation above the energy threshold of 11.2 eV can dissociate H₂ in 2H, but harder photons with energies larger than 15.42 eV would simply ionize the residual H₂ into H⁺ + e⁻ (see Table 2). Also, for H₂⁺, there are two possible branches: one above an energy threshold of 2.65 eV and below 21 eV (H₂⁺ + γ → H⁺ + H), and a second between 30 and 70 eV (H₂⁺ + γ → 2H⁺ + e⁻). For the HeH⁺ radiative interaction considered in our network, the energy threshold is about 1.7 eV.

The set of differential equations (equation 5) is integrated via simple linearization. So, given the time-step \(\Delta t\), at each time \(t\) the temporal variation of the number fraction of species \(i\) can be written as

\[
\frac{n_i(t + \Delta t) - n_i(t)}{\Delta t} = C_i^i + \Delta t - D_i^i + \Delta t n_i(t) + \Delta t, \tag{8}
\]

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3 TEST SIMULATIONS

In order to test the implementation, we perform numerical simulations under different conditions. First, we numerically solve an expanding ionized sphere problem (Section 3.1) by fully including both the RT and chemistry treatments. Then, we show the cosmic evolution of the different chemical species, coupled with the radiative gas emissions (Section 3.2). Finally, we perform cosmological simulations of early structure formation (Section 4) to check the effects of radiative feedback on gas cooling and collapse.

For all simulations, we use a set of 284 frequencies, covering the range 0.7–100 eV. The density of frequency bins around the peaks of the photoionization and photodissociation cross-sections is increased (i.e. there are more frequency bins in the spectral regions of interest). In this way, we can ensure that photons are both traced and absorbed properly and no spectrum-averaging mistakes are made.

3.1 Ionized sphere expansion

3.1.1 Ionized sphere expansion in a static density field

The expansion of an I-front in a static, homogeneous and isothermal gas is the only problem in radiation hydrodynamics that has a known analytical solution. Therefore, it is the most widely used test for RT codes (e.g. Iliev et al. 2006, 2009). For such a set-up, the ionized bubble around the ionizing source reaches a final steady radius, called the Str"omgren radius, where absorptions and recombinations are balanced along the line of sight. For an H-only gas, the Str"omgren radius is analytically given by

\[ r_S = \left( \frac{3N_{\gamma}}{4\pi\sigma_0 n_H} \right)^{1/3}, \]

where \( N_{\gamma} \) is the luminosity of the source in photons per second, \( \sigma_0 \) is the case B recombination coefficient and \( n_H \) is the hydrogen number density. The case B recombination coefficient assumes the so-called ‘on-the-spot’ approximation, where photons from recombinations to lower energy levels are immediately absorbed in the vicinity of their emission (e.g. Spitzer 1978). If we approximate the I-front as infinitely thin (i.e. it features a discontinuity in the ionization fraction), the temporal expansion of the Str"omgren radius can be solved analytically in closed form, with the I-front radius \( r_t \) given by

\[ r_t = r_S [1 - \exp(-t/t_{rec})]^{1/3}, \]

where

\[ t_{rec} = \frac{1}{n_H \sigma_0} \]

is the recombination time.

In our first test, we perform an ionized sphere expansion, but we allow the temperature of the gas to vary in order to test the coupling between the RT and the full non-equilibrium chemistry treatment. As a reference, we compare the analytical case with constant temperature. We follow the expansion of an ionized sphere around a source that emits \( N_{\gamma} = 5 \times 10^{46} \) photons s\(^{-1}\). The shape of the source spectrum corresponds to a \( 3 \times 10^2 \) K blackbody. The surrounding gas density is \( \rho = 1.7 \times 10^{-27} \) cm\(^{-3}\) \((\sim 10^{-3} \text{ cm}^{-3})\) and this is sampled by 16\(^2\), 32\(^2\) and 64\(^2\) gas particles.\(^1\) In the 32\(^2\) case, the shielding of Draine & Bertoldi (1996) has also been adopted, with the values cited in their paper. The initial temperature of the gas is set to \( T = 10^2 \) K, and this is subject to photoheating and radiative cooling. At a temperature of \( 10^5 \) K, the case B recombination coefficient is \( \sigma_0 = 2.59 \times 10^{-13} \) cm\(^3\) s\(^{-1}\) (e.g. Iliev et al. 2009). Given these parameters, the recombination time is \( t_{rec} = 125,127 \) Myr, and the expected Str"omgren radius in the isothermal case (assuming \( T = 10^2 \) K) is \( r_S = 5.4 \) kpc.

Fig. 2 shows the evolution of the radial position of the I-front with time for the different resolutions. As a proxy for the position of the front, we take the radius where the neutral and ionized hydrogen fractions are equal (see also Fig. 3).

All resolutions agree very well with each other. There is no difference in the case with shielding because the simulation never reaches the densities required to produce some effect, as discussed in the introduction. Our results agree within 10 per cent with the analytical results from equation (15). In particular, the simple analytical solution is systematically larger than the full-simulation trend, which is expected. This can be explained by the missing cooling contributions in the analytical calculations from, for example, He, H\(_2\), H\(_3^+\) and HD, which lower temperatures, enhance recombination and make the Str"omgren radius decrease (as is visible in the simulated case). In fact, equation (15) is computed by assuming constant

\(^1\) For more resolution studies, see Petkova & Springel (2009), who show that numerical convergence is already reached with 8\(^3\) particles.
temperature for hydrogen-only gas (see also Petkova & Springel 2009). In the numerical calculations, the full chemistry treatment of Table 2, including cooling and heating, is considered. Pawlik & Schaye (2011) find similar results in their one-dimensional ionized sphere simulations.2

Fig. 3 shows the radial profile of the temperature of the gas at 500 Myr after the source has been switched on. The temperature inside the ionized region reaches \( \sim 10^{4} \) K, consistent with photoheating from a stellar-type source, and it extends beyond 5 kpc. Even further, the temperature begins to drop. Harder photons (with energies \( \geq 60 \) eV), which do not ionize the elements effectively, heat the medium ahead of the I-front. If the source had a harder spectrum (e.g. \( 10^{5} \) K blackbody), then the gas would be heated even at larger radii. We stress that at a distance of \( \gtrsim 5 \) kpc (i.e. around the Strömgren radius) temperatures drop steeply from \( \sim 10^{4} \) K down to \( \sim 10^{1} \) K and recombination processes take place.

With respect to the temperature profile, in Fig. 3, we display the radial profiles of the different chemical abundances at 500 Myr after the radiative source has been switched on. We have assumed initial cosmic abundances,3 which means that hydrogen species account for \( \sim 93 \) per cent of the total number densities, and that helium species account for \( \sim 7 \) per cent. As expected, ionized fractions usually have larger values closer to the sources (within a few kpc), while neutral or molecular fractions increase at larger distances (above 3–6 kpc). In the following, by referring to the reaction network of Table 2, we discuss these trends in a more precise and detailed way.

(i) Atomic hydrogen species. Because of the strong radiation intensities near the central source, hydrogen is kept completely ionized (i.e. the total hydrogen fraction, \( \sim 0.93 \), is in the ionized state, \( \text{H}^{+} \)) within \( r \lesssim 5 \) kpc by the dominant photoionization process:

\[
\text{H} + \gamma \rightarrow \text{H}^{+} + e^{-}.
\]

Only at larger radii, where the radiation intensity decreases, does the recombination process

\[
\text{H}^{+} + e^{-} \rightarrow \text{H} + \gamma
\]

take over and make the \( \text{H}^{+} \) fraction drop down by several orders of magnitude, with the consequent increase of the H fraction up to \( \sim 0.93 \) (i.e. the total hydrogen fraction is now in the neutral state).

\( \text{H}^{-} \) is a very important species because it represents one of the main channels by which molecular hydrogen can be formed [see the discussion (iv)]. It shows fractional values of \( \sim 10^{-9} \sim 10^{-10} \) until \( r \lesssim 6 \) kpc and, at larger distances, it shows drops of roughly 3–4 orders of magnitude. The increment of the \( \text{H}^{-} \) fraction up to \( \sim 10^{-9} \) corresponding to \( r \sim 4–5 \) kpc is a result of the simultaneous hydrogen recombination (equation 18), which leads to an increase of the neutral hydrogen and enhances the \( \text{H}^{-} \) formation via

\[
\text{H} + e^{-} \rightarrow \text{H}^{-} + \gamma
\]

reaction. In the innermost regions, because of the low ionization energy of only 0.755 eV, \( \text{H}^{+} \) photoionization

\[
\text{H}^{+} + \gamma \rightarrow \text{H} + e^{-}
\]

and collisional destruction by the abundant \( \text{H}^{+} \) and \( e^{-} \) species

\[
\text{H}^{-} + \text{H}^{+} \rightarrow 2\text{H}
\]

\[\text{equation (15).} \]

\[\text{Note that Pawlik & Schaye (2011) adopt a blackbody spectrum with an effective temperature of } 10^5 \text{ K, and therefore they produce different temperature and He radial profiles.} \]

\[\text{These are set to } x_{\text{He}} = 4 \times 10^{-4}, x_{\text{H}} = 0.926, x_{\text{HI}} = 4 \times 10^{-4}, x_{\text{HeI}} = 10^{-19}, x_{\text{HeII}} = 0.07, x_{\text{HeIII}} = 10^{-25}, x_{\text{HeIV}} = 10^{-30}, x_{\text{H}} = 10^{-13}, x_{\text{He}}^4 = 10^{-18}, x_{\text{HeD}} = 10^{-16}, x_{\text{D}} = 10^{-5}, x_{\text{DP}} = 10^{-7} \text{ and } x_{\text{HeH}^+} = 10^{-21}. \]

\[\text{Fig. 2. Evolution of the radial position of the I-front. The smooth (red) line shows the analytical solution for an isothermal hydrogen-only sphere. The black lines show our results from the simulations, assuming the radius is at the position where the amounts of neutral and ionized hydrogen are equal. The thick dashed line, the thinner dash-dotted line and the thin solid line show the results from the simulations with } 64^2, 16^2 \text{ and } 32^2 \text{ particles, respectively. In the simulation with } 32^2 \text{ particles, H}_2 \text{ shielding has also been adopted. All lines agree very well with each other, where the lowest resolution exhibits more scatter. The results from the simulation with shielding show that it can be discarded in set-ups like this, where no high particle number densities are reached. As shown in other studies (see text), the radius of the I-front always remains below the analytical solution given by equation (15).} \]

\[\text{Fig. 3. Top panel: chemical abundance fraction radial profiles at 500 Myr after the source has been switched on. Bottom panel: temperature radial profiles at 500 Myr after the source has been switched on. The temperature inside the ionized region reaches } \sim 10^4 \text{ K and extends beyond 6 kpc because harder photons, unabsorbed by the gas, heat the medium ahead of the I-front. All simulations with different resolutions and shielding agree very well with each other, at all radii.} \]
\[ H^- + H^+ \rightarrow H_2 + e^- \]  \hspace{1cm} (22) \\
\[ H^- + e^- \rightarrow H + 2e^- \]  \hspace{1cm} (23)

determine a lower fraction of \( \sim 10^{-10} \). At larger distances (\( r \sim 5-10 \) kpc), \( H \) is dominant. However, contrary to reaction (19), free \( e^- \) are lacking and the most effective reactions are
\[ H^- + H \rightarrow H_2 + e^- \]  \hspace{1cm} (24) \\
\[ H^- + H \rightarrow 2H + e^- \] \hspace{1cm} (25)

which lead to a decrease of the \( H^- \) fraction to \( \lesssim 10^{-13} \).

We note that a calculation of the exact analytical expression for the the Strömgren radius and a comparison with our results are not meaningful, because the analytical study is based on the simplified case of hydrogen-only gas and it does not take into account the interaction with other species and the effects of photoheating. However, the radius of the ionized hydrogen reaches \( \sim 5 \) kpc, which is approximate to the expected value of the Strömgren radius for the isothermal case.

(ii) Atomic helium species. In the same way, because of the reactions
\[ He + \gamma \rightarrow He^+ + e^- \]  \hspace{1cm} (26) \\
\[ He + e^- \rightarrow He^+ + 2e^- \] \hspace{1cm} (27)

neutral \( He \) is efficiently destroyed at \( r \lesssim 3 \) kpc, and the residual fraction is \( \sim 0.01 \). \( He^+ \) and \( He^{++} \) reach fractions of \( \sim 0.06 \) and \( \sim 10^{-5} \), respectively, via
\[ He^+ + e^- \rightarrow He^{++} + 2e^- \] \hspace{1cm} (28) \\
\[ He^+ + \gamma \rightarrow He^{++} + e^- \] \hspace{1cm} (29)

and
\[ He^{++} + e^- \rightarrow He^+ + \gamma \]  \hspace{1cm} (30)

Moreover, the additional \( He \) depletion by \( H^+ \) collisions leads to the formation of \( HeH^+ \) (as we discuss later). At \( r > 3 \) kpc, the decreasing intensity of ionizing radiation, which plays the most relevant role in equations (26) and (29), and the ongoing recombination processes, which take away free electrons from the medium, needed, for example, in reactions (27) and (28), cannot sustain ionization any longer, and the trends exhibit monotonic radial drops for both \( He^+ \) and \( He^{++} \). More exactly, \( He^+ \) and \( He \) recombine according to
\[ He^{++} + e^- \rightarrow He^+ + \gamma \]  \hspace{1cm} (31) \\
and
\[ He^+ + e^- \rightarrow He^+ + \gamma \] \hspace{1cm} (32)

respectively. So, the final states of \( He^+ \) and \( He^{++} \) are strictly linked to each other with abundances of \( \sim 10^{-5} \) and \( 10^{-11} \) at \( r \sim 8 \) kpc. Radiative interactions are weaker and weaker, and they become practically negligible at large radii.

(iii) Atomic deuterium species. The behaviours of \( D \) and \( D^+ \) are quite regular and they are similar to those of \( H \) and \( H^+ \), with \( D^+ \) being dominant at \( r \lesssim 5 \) kpc and \( D \) being dominant at \( r > 5 \) kpc, reaching a difference of 3 orders of magnitude at \( r \sim 8 \) kpc. The abundances of the deuterium and hydrogen species are bound by the balance reactions
\[ H^+ + D \rightarrow H + D^+ \] \hspace{1cm} (33) \\
\[ H + D^+ \rightarrow H^+ + D. \] \hspace{1cm} (34)

and
\[ H + D \rightarrow HD + H. \] \hspace{1cm} (35)

However, the most efficient processes are still photoionization (‘close’ to the source)
\[ D + \gamma \rightarrow D^+ + e^- \] \hspace{1cm} (36)

and recombination (‘far’ from the source)
\[ D^+ + e^- \rightarrow D + \gamma. \] \hspace{1cm} (37)

Minor contributions of \( D \) and \( D^+ \) are also involved for molecular species [see (iv)] and these can slightly affect \( H \) or \( H^+ \) production.

(iv) Molecular species. Finally, we discuss the trends of molecular species (\( H_2, H_2^+, HD \) and \( HeH^+ \)). Their profiles are less regular and intuitive than atomic profiles, because more processes need to be addressed at the same time. For example, \( H_2 \) and \( H_2^+ \) have fractional values of \( \sim 10^{-13} \) and \( \sim 10^{-10} \), respectively, at \( r \sim 1 \) kpc. Then, they show an increasing trend and a peak of \( \sim 10^{-10} - 10^{-9} \) at \( r \sim 4-6 \) kpc. For larger \( r \), they exhibit a drop off below \( \sim 10^{-14} \), with \( H_2 \) overcoming \( H_2^+ \) at \( r > 7 \) kpc. These behaviours are understood by considering that, in the innermost regions, the radiative negative feedback on molecular formation decreases for increasing \( r \); this means that, at larger radii, radiation is not strong enough to dissociate molecules via
\[ H_2 + \gamma \rightarrow 2H. \] \hspace{1cm} (38)

Also, because of the available \( H, H^+ \) and \( e^- \) (simultaneously present at \( r \sim 4-6 \) kpc, where \( H \) recombination is still taking place), \( H_2 \) formation can proceed through the \( H^- \) channel (see also reaction 19),
\[ H + e^- \rightarrow H^- + \gamma. \] \hspace{1cm} (39) \\
\[ H^- + H \rightarrow H_2 + e^- \] \hspace{1cm} (40)

and through the \( H_2^+ \) channel,
\[ H + H^+ \rightarrow H_2^+ + \gamma. \] \hspace{1cm} (41)

\( H_2^+ + H \rightarrow H_2 + H^+ \) and through the \( H_2^+ \) channel,
\[ H + H^+ \rightarrow H_2^+ + \gamma. \] \hspace{1cm} (42)

This is the intrinsic reason why molecular hydrogen roughly follows the \( H^- \) profile discussed earlier. Obviously, residual photons will slightly boost the ionized fraction of \( H_2^+ \) (with respect to \( H_2 \)) via
\[ H_2 + \gamma \rightarrow H_2^+ + e^- \] \hspace{1cm} (43)

until \( r \sim 7 \) kpc. At larger distances, photons are too weak to ionize the gas, so \( H_2 \) takes over and \( H_2^+ \) drops dramatically by \( \sim 3 \) orders of magnitude within 1 kpc. Additionally, we note that the sharp decrement of molecular fractions at very large distances is basically because the medium becomes almost completely neutral and the ionized fractions of \( e^- \) and \( H^+ \) are too low to boost \( H^- \) and \( H_2^+ \), and hence \( H_2 \) formation.

Similarly, the increase with the radius of the HD fraction is essentially caused by the weakening of the central radiation and of \( H^+ \) and \( e^- \) fractions, which are less and less effective at dissociating it at larger \( r \). In particular, at \( r \lesssim 4 \) kpc, \( H, D \) and \( H_2 \) are subdominant with respect to their ionized counterparts \( H^+, D^+ \) and \( H_2^+ \). Thus, HD formation as a result of
\[ D + H \rightarrow HD + H \] \hspace{1cm} (44)

is strongly inhibited, while little contributions come from
\[ D^+ + H \rightarrow HD + H^+. \] \hspace{1cm} (45)
Further lowers HD abundances around the $\sim 10^{-18}$ level. At $r \gtrsim 4$ kpc, hydrogen and deuterium recombinations, together with H$_2$ formation via the H$^+$ channel, support HD formation through reactions (43) and (44), because reaction (45) is no longer effective. As a consequence, the HD fractional abundance grows by more than $\sim 2$ orders of magnitude at $r \sim 8$ kpc. We note that a boost of HD production in shock-compressed gas was expected because of the simultaneous increment of H$_2$ fractions, quite visible in Fig. 3, corresponding to the Strömgren radius.

Concerning the aforementioned HeH$^+$, this is efficiently produced near the source because there are many free protons that can boost its abundance via

$$\text{He} + \text{H}^+ \rightarrow \text{HeH}^+ + \gamma,$$

(46)
even in a more powerful way than photodissociation

$$\text{HeH}^+ + \gamma \rightarrow \text{He} + \text{H}^+.$$  

(47)

Only when protons are lacking (i.e. at large $r$) is HeH$^+$ production inhibited up to $\sim 3$ orders of magnitude, and it drops from $\sim 10^{-11}$ to $\sim 10^{-14}$.

We note that the residual relative ionized fractions far from the source ($r \sim 8$ kpc) are $n_{\text{H}^+}/n_{\text{H}_2} \sim 10^{-3}$, $n_{\text{D}^+}/n_{\text{D}_2} \sim 10^{-3}$, $n_{\text{He}^+}/n_{\text{He}_2} \sim 10^{-4}$, $n_{\text{H}_2^+}/n_{\text{H}_2^3} \sim 10^{-3}$, $n_{\text{He}_2^+}/n_{\text{He}_2^3} \sim 10^{-9}$ and $n_{\text{H}_3^+}/n_{\text{H}_3^4} \sim 10^{-1}$. The absolute values quoted in the previous discussion are dependent on the initial composition assumed for the gas. Although the qualitative behaviour is not supposed to change much, larger or smaller values for the assumed fractions could result in more efficient or less efficient formation and destruction processes, respectively. However, the general trends are supposed to be independent of this.

The test presented here is based on the initial conditions of Iliev et al. (2009), but there are others available in the literature. In fact, similar results in the same direction have been found by, for example, Ricotti et al. (2001), Ahn & Shapiro (2007) and Whalen & Norman (2008), who independently developed different H, He and H$_2$ chemistry networks. However, their simulation set-ups were very different, as well as the parameters for the central source.

Ricotti et al. (2001) performed the first one-dimensional calculations of a star shining in a primordial mini-halo (see their fig. 3). A popIII-like source with a power-law spectrum and $N_{\gamma}$ $\sim 1.2 \times 10^{48}$ s$^{-1}$ at $z \sim 19$ was located in a static, uniform medium at the mean density $n(z \sim 19) \sim 0.1$ cm$^{-3}$. They studied the behaviour of the molecular species after $\sim 100$ Myr from the explosion of the central star, when the Strömgren radius had reached $\sim 4$ kpc, and a corresponding peak of H$_2$ had formed with $x_{\text{H}_2} \sim 5 \times 10^{-2}$, a few kpc wide. This was equivalent to a boost of about three orders of magnitude with respect to the initial $x_{\text{H}_2} \sim 10^{-6}$ value assumed. In our previous discussion, despite the different initial values, we have also found an increase in the H$_2$ fraction of $\sim 3$ orders of magnitude.

Similarly, Ahn & Shapiro (2007) (see their fig. 8) and Whalen & Norman (2008) (see their fig. 1) performed one- and three-dimensional calculations, respectively, considering a 120-M$_\odot$ popIII-like source with a blackbody spectrum that has an effective temperature of $T_{\text{eff}} = 10^4$ K and $N_{\gamma} \sim 1.5 \times 10^{48}$ s$^{-1}$. They assumed that the star was in a primordial halo with a truncated isothermal sphere density profile, whose central matter densities were reaching up $\gtrsim 4 \times 10^{-22}$ g cm$^{-3}$. They focused on the innermost core of the star-forming regions, after roughly 0.6 times the lifetime of the massive popIII stars (a few Myr), when the Strömgren radius was still around $\lesssim 30$ pc and a corresponding peak of H$_2$ of $\sim 10$ pc wide, had arisen. They also found an increase to $x_{\text{H}_2} \sim 10^{-4}$, a few orders of magnitude larger than the assumed initial value of $x_{\text{H}_2} \sim 10^{-6}$.

The first relevant difference with our study is in the assumed $N_{\gamma}$ (our value is $5 \times 10^{48}$ s$^{-1}$): Ricotti et al. (2001) used a value of $N_{\gamma}$ 2.2 times larger, while Ahn & Shapiro (2007) and Whalen & Norman (2008) used a value 300 times larger. Consequently, the number of photons available to ionize atoms or dissociate molecules is much larger in their cases than in ours. This explains why they have found H$_2$ fractions more significantly destroyed in the inner regions.

Thus, molecular dissociation or creation is also strictly linked to the typical conditions of the medium. In the aforementioned works, these are denser than in our study (by $\sim$ two to four orders of magnitude). This has strong implications when computing abundances, because higher densities allow easier collisional dissociation in the inner, ionized regions. When temperatures fall below $\sim 10^4$ K, the creation of H$_2$ becomes more efficient and larger free-electron number densities can lead to a noticeable increase of molecular fractions. This is actually the reason why the profiles of our low-density gas in Fig. 3 show H$_2$ increases up to only $\sim 10^{-6}$, while very overdense gas can reach H$_2$ fractions of $\sim 10^{-4}$ in front of the propagating I-front.

We conclude by noting that, despite the huge diversities in the parameters and in the H$_2$ peak values, the different behaviours of the profiles are in qualitative agreement, showing an increment of the molecular fractions corresponding to the I-front and orders-of-magnitude declines farther away. Together with the H$_2$ rise (within a shell of $\sim 2$ kpc) the consequent HD increment is obviously expected to be more prominent in high-density environments.

None the less, the final effects for the triggering of star formation are not completely clear, because gas runaway collapse can be significantly enhanced only when densities are larger than $\sim 10^2$ cm$^{-3}$, and molecular fractions increase up to $\sim 10^{-2}$ (see further discussion in Section 4).

### 3.1.2 Ionized sphere expansion in a dynamic density field

In this section, we repeat the test from the previous section, but we allow the gas particles to move as a result of pressure forces, but not gravity. The density field is no longer static. The resolution we have chosen here is $32^3$ gas particles.

The position of the I-front at this stage is given by (Spitzer 1978)

$$r_{\text{I}} = r_{\text{S}} \left( 1 + \frac{7c_s t}{4r_{\text{S}}} \right),$$  

(48)

where $c_s$ is the sound speed of the ionized gas and $r_{\text{S}}$ is the Strömgren radius given by equation (15).

Fig. 4 shows the evolution of the position of the I-front and its velocity with time. We compare the analytical results from equations (15) and (48). We note that the I-front follows the analytical prediction for static gas in the beginning of the expansion. After approximately 200 Myr, at approximately 5 kpc from the source, the I-front continues to move outwards, rather than starting to decelerate, and it follows the dynamic gas solution equation (48).

---

4 For example, electron fractions of $\sim 10^{-4}$ determine typical intergalactic medium (IGM) fractions of H$_2$ of $\sim 10^{-6}$. However, in gas with overdensities of $\sim 10^3$, H$_2$ fractions can be boosted up to $\sim 10^{-4}$ (Ahn & Shapiro 2007).
Evolution of the radial position of the I-front. The unsmooth line shows our results from the simulation, assuming the radius is at the position where the amount of neutral and ionized hydrogen is equal. The solid line is the result from equation (15), computed by assuming isothermal gas at $10^4$ K. The extension of the solid line is given by equation (48). The results from the simulation agree very well with the analytical results, also at radii beyond the Strömgren radius $r_s$.

Fig. 5 presents the radial profiles of the different species, the temperature and the density of the gas at $t = 200$ Myr after the source has been switched on. The temperature in the ionized sphere is $\sim 10^4$ K, and there is a shock and a density contraction ahead of the I-front that moves at supersonic speed at this evolution time. We also note that there are also an HD boost and an H$_2$ shell ahead of the I-front, inside the density contraction region. Similar results have also been shown by Ricotti et al. (2001). These conditions (i.e. increased density and increased H$_2$ fraction) are favourable for star formation.

### 3.2 Cosmological abundance evolution

In order to test how our implementation performs during cosmological evolution, we run the chemical network coupled with the RT network for the mean background density evolution and we follow the changes in the different species as a function of the cosmic time. The radiative source is assumed to be the uniform cosmic microwave background (CMB) radiation with a blackbody spectrum with an effective temperature of $\sim 2.73(1+z)$ K. The CMB radiation is self-consistently followed, according to the treatment outlined in Section 2.

The initial fractions, $x$, for the different species\textsuperscript{5} are initialized, at redshift $z \simeq 10^5$, according to a neutral plasma at $\sim 10^4$ K (see, for example, Galli & Palla 1998).

We present the results in Fig. 6, where the cosmic mean number fractions as a function of redshift are plotted for a standard flat ΛCDM cosmology with geometrical parameters $\Omega_{\rm{tot}} = 1.0$, $\Omega_{\Lambda} = 0.7$, $\Omega_{\rm{b}} = 0.3$ and $\Omega_{\rm{b}} = 0.04$. The H and He number fractions are unaffected by the redshift evolution.

At early times, some residual recombination processes continue to take place, while the CMB temperature decreases, and these make H\textsuperscript{+} evolution drop from a fraction of $\sim 10^{-3}$, at $z \sim 1000$, to the final value of $\lesssim 10^{-4}$. The evolution of H\textsuperscript{+} clearly shows the effects of free electrons at high redshift, which boost its formation (and H-derived molecular formation) from $x_{\text{HI}} \sim 10^{-20}$, at $z \sim 1000$, to $x_{\text{HI}} \sim 10^{-12}$, at $z \sim 100$. The following hydrogen recombination implies a decrease in both H\textsuperscript{+} and e\textsuperscript{-} fractions, with a consequent drop of H\textsuperscript{+} (see Table 2) to $x_{\text{HI}} \sim 10^{-15}$ at low redshift. The two ionization states of He are constantly kept at very low values, close to the initial values (their trends are not displayed in Fig. 6 for the sake of clarity).

As already mentioned, hydrogen molecular formation is initially enhanced because of the available residual e\textsuperscript{-} and the progressively diminishing effects of CMB radiation. This allows hydrogen to increasingly form H$_2$, with a peak around $z \sim 300$, and H$_2$, until $z \sim 70$. H$_2$ formation is efficiently driven by H and the available H\textsuperscript{+} in primordial times. At $z \lesssim 300$, the paucity of free protons (whose fraction in the mean time has dropped by about one order of magnitude) makes H$_2$ formation difficult. However, the continuous increment of H\textsuperscript{-} enhances H$_2$ at $z \sim 100$, and afterwards its formation is mainly driven by the H\textsuperscript{-} channel, rather than the H$_2$ channel, until $z \sim 70$. The dominant formation path at different times is clearly recognizable when comparing the H$_2$ trend with the H\textsuperscript{+} and H\textsuperscript{-} trends. The $z \sim 300$ peak of H$_2$ corresponds to the steep increase of $x_{\text{HI}}$ at early times, while the $z \sim 100$ peak of H\textsuperscript{-} corresponds to the following boost at later times. For $z \lesssim 70$, $x_{\text{HI}}$ remains roughly constant between $10^{-7}$ and $10^{-6}$, because further production is halted by the decrement of free protons and electrons.

\textsuperscript{5} These are set to $x_{\text{e}} = 4 \times 10^{-4}$, $x_{\text{HI}} = 0.926$, $x_{\text{H}\text{+}} = 4 \times 10^{-4}$, $x_{\text{H}\text{++}} = 10^{-19}$, $x_{\text{He}^+} = 0.07$, $x_{\text{He}\text{++}} = 10^{-25}$, $x_{\text{He}\text{+++}} = 10^{-30}$, $x_{\text{He}} = 10^{-13}$, $x_{\text{H}_2} = 10^{-18}$, $x_{\text{H}_2}\text{D} = 10^{-16}$, $x_{\text{D}} = 10^{-5}$, $x_{\text{He}\text{+}} = 10^{-2}$ and $x_{\text{He}\text{++}} = 10^{-21}$.

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and radiative destruction cannot take place because of the low CMB flux at low redshift.

Deuterium is also affected by cosmological evolution and the weaker CMB intensity effects at lower redshift. Thus, the recombination of D and D\(^+\) makes x_D increase up to \(\sim 10^{-4}\) and it makes x_D\(^+\) drop dramatically at \(z < 100\). The simultaneous ongoing H\(_2\) formation at \(z \geq 70\) also ‘drags’ HD fractions up to \(\sim 10^{-9}\) levels (HD is very sensitive to H\(_2\) abundances).

The HeH\(^+\) molecule is often formed behind fast shocks (e.g. Neufeld & Dalgarno 1989) by He and H\(^+\). However, because of its low dissociation energy (of \(\sim 14.873\) eV; Bishop & Cheung 1979), it can be found and emitted only below \(\sim 10^4\) K. Moreover, the presence of background radiation can dissociate it into its two components soon after the recombination epoch, at \(z \lesssim 10^1\). Indeed, the plot in Fig. 6 highlights how HeH\(^+\) is initially underabundant, and then is gradually formed while the Universe expands and cools and the CMB radiation becomes weaker. Over the cosmic time, x_{HeH^+} slightly increases by one order of magnitude, from \(\sim 10^{-14}\) to \(\sim 10^{-13}\). Because of H interactions, it sustains H\(_2\) with subsequent H\(_2\) formation.

The low radiation intensity of the CMB is not able to produce large changes in the abundances of the elements, but it is nevertheless a good test for the performance of our implementation. Our results agree very well with previous cosmological abundance evolution studies, such as, for example, Abel et al. (1997), Galli & Palla (1998) and Maio et al. (2007).

The presence of additional cosmic UV radiation during reionization (e.g. Haardt & Madau 1996) at low redshift (\(z \lesssim 7\)) would heat the medium and change the ionization equilibria. As a consequence, we might expect more free electrons, larger H\(_2\) and H\(^+\) abundances, and hence more H\(_2\) production, accompanied by increased D\(^+\) and HD fractions, and the dissociation of HeH\(^+\).

4 APPLICATION: COSMOLOGICAL STRUCTURE FORMATION

As a final application, we present the results from simulations of a cosmological structure formation in the framework of the standard \(\Lambda\)CDM model. We also consider additional feedback mechanisms from star formation (as already mentioned in Section 1). We use a periodical comoving box size of \(L_{\text{box}} = 0.5\) h\(^{-1}\) Mpc on a side with \(2 \times 64^3\) gas and dark matter particles (for a resulting spacial resolution of \(\sim 0.4\) kpc h\(^{-1}\) comoving), sampled at the initial redshift \(z = 100\). The runs include gravity, hydrodynamics, wind feedback, non-equilibrium chemistry and radiative transfer. Stars are taken to be sources of ionizing radiation. Because each star particle in the simulation represents a whole stellar population with a Salpeter distribution, about 12 per cent of its mass is in high-mass stars (\(\gtrsim 10\) M\(_{\odot}\)) that are able to produce UV photons. The frequency distribution is assumed to be a blackbody spectrum with an effective temperature of \(3 \times 10^4\) K, which corresponds to a luminosity of \(8 \times 10^{48}\) photons s\(^{-1}\) per high-mass star in the stellar population of the star particle. We assume that gas particles are converted into stars once a critical density of \(\sim 10^{-2}\) cm\(^{-3}\) is reached, and the gas temperature is below \(\sim 10^4\) K, to make sure that the gas is effectively cooling (see details in Maio et al. 2009). Star-forming particles also experience supernova-explosion feedback, which heats the gas above \(\sim 10^4\) K, and wind feedback, which expels gas with a typical velocity of \(\sim 500\) km s\(^{-1}\) (see also Springel 2005, and references therein).

A pictorial representation of the simulated box is given in Fig. 7, where we show mass-weighted temperature slices through the simulation volume at redshifts \(z = 10.61\) and \(z = 6.14\). For the full run, including, in particular, both non-equilibrium chemistry and RT.

The first sources are clearly visible close to the central part of the slice. While the structure growth proceeds, more sources are found in scattered places along the converging filaments. Obviously, in a wider perspective (i.e. on a \(\sim 100\)-Mpc scale), radiative sources would be much more uniformly distributed. However, there are currently serious computational limitations for performing simulations with such large box sides and, simultaneously, with a resolution good enough to resolve chemical evolution and radiative transfer at the same time. In the maps, the filamentary cold structures led by early molecular gas are clearly visible at temperatures around hundreds of Kelvin. In the densest regions, radiative effects from the first stars already heat the medium above \(\sim 10^4\) K by redshift \(z \sim 10\). More and more star formation episodes appear at later stages and these contribute to the cosmic reionization process down to redshift \(z \gtrsim 6\).

Given the small size of our box, we can clearly focus on the infalling phases of the cold material in the intersection of primordial filamentary structures, and on the subsequent supernova explosions, which heat the gas and push material into the lower-density, void regions. This helps us to understand the different roles played by the various feedback mechanisms. However, the lack of a very large box also leads to an insufficient number of stellar sources to fully complete reionization by \(z \sim 6\).

In Fig. 8, we plot the phase diagrams (gas temperature versus number density) for the simulations with and without radiative treatment. The shading shows the mass fraction of H\(_2\). Molecular hydrogen is dissociated in the presence of ionizing radiation (mostly in the LW band), and this effect increases with decreasing redshift, because of the higher number of available photons. As a consequence, this lowers the star formation process, because H\(_2\) provides the largest part of the cooling below \(10^4\) K. It is evident from the plots that without radiative feedback H\(_2\) can reach levels \(\gtrsim 10^{-2}\) and that it can boost early star formation. In the presence of radiation from stellar sources, molecular fractions decrease by several orders of magnitude to \(\lesssim 10^{-4}\). This effect is stronger for low-density gas, where molecules re-form more slowly. Such behaviour is clear from both cases shown, at redshifts \(z = 10.61\) and \(z = 6.14\). In the latter case, a wider temperature spread, as a result...
Radiative feedback and cosmic molecular gas

Figure 7. Mass-weighted temperature slices through the box at redshifts $z = 10.61$ (left) and $z = 6.14$ (right). The simulation includes feedback effects, full non-equilibrium chemistry and RT (see text).

Figure 8. Phase diagrams: temperature versus gas comoving number density at redshifts $z \sim 10$ (top) and $z \sim 6$ (bottom) for a simulation without (left) and with (right) ionizing radiation. The shading shows the mass fraction of H$_2$. In the presence of ionizing radiation, H$_2$ is depleted on all scales by many orders of magnitude. The effect is stronger at lower redshift because of the larger number of photons available.

The lack of very cold gas in the more realistic case with both chemistry and RT suggests that low-temperature cooling by metals (e.g. Maio et al. 2007) could be an important mechanism to sustain star formation after the generation of the first stars (Maio et al. 2010). To better underline the impacts of radiative effects on early

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6 We could also rely on reionized gas (Yoshida et al. 2007) to form subsequent baryonic structures.
chemistry, we also show in Fig. 9 the redshift evolution of the mean and maximum number fractions of the two main molecules, H$_2$ and HD, and of the basic species for the different channels of molecular formation, H$^-$ and H$_2^+$. As mentioned previously, after early star formation sets in, around redshift $z \sim 12$, the H$_2$ fraction drops by several orders of magnitude (from average values of $\sim 10^{-5}$ to $\lesssim 10^{-10}$), as ionizing radiation starts to propagate in the simulated volume. This is not seen in the case without radiation, where H$_2$ increases almost monotonically, with peak values of $\sim 10^{-3}$ at $z \approx 6$.

The mean HD fraction remains roughly constant in the presence of ionizing radiation, but it is increasing in the case without radiation. When comparing peak values, we see that, at $z \approx 12$, HD has fractions of $\sim 10^{-6}$ in both cases but, in the RT case, it is significantly destroyed when photons begin to propagate. Instead, in the non-RT case, its maximum values catch up with H$_2$.

The H$^-$ fraction is crucial for H$_2$ formation via the H$^-$-channel. In the presence of RT, its mean values are lowered to $\sim 10^{-12}$, so they cannot catalyse further molecular formation efficiently. In the non-RT case, H$^-$ would increase by two orders of magnitude.

Similarly, H$_2^+$ catalyses H$_2$ formation via the H$_2^+$-channel, but photon propagation destroys molecules and inhibits H$_2$ formation. As a comparison, in the non-RT run, H$_2^+$ reaches mean values of $\sim 10^{-10}$, a couple of orders of magnitude larger than in the RT run. Maximum fractions for H$^-$ and H$_2^+$ are similarly suppressed by about one order of magnitude.

As a conclusion, the radiative feedback is responsible for molecular dissociation. Molecules are easily depleted, not only from the external sources, but also from the central sources that have just been formed. This is justified by the fact that catastrophic molecular cooling has already set in at densities $\gtrsim 1$ cm$^{-3}$ when the material is optically thin. Thus, there is no significant gas shielding preventing H$_2$ and HD dissociation. In fact, in the simulations presented here, radiative feedback becomes effective at densities $> 10$ cm$^{-3}$. In the innermost central regions (i.e. below a few hundreds of comoving parsec, not sampled by our simulations because of resolution limits), densities could rise up to values greater than $\sim 10^5$ cm$^{-3}$, they could become optically thick and they could produce significant shielding. However, this should not affect the overall molecular destruction over $\sim$ kpc scales by external sources.

We stress that precise, quantitative assessments about the net effects of radiative feedback on the surrounding gas are difficult, because it should be possible to prove RT on very different scales within N-body/hydrochemistry calculations. While the destruction of molecules in low-density IGM is intuitive and expected, the behaviour in the innermost cores of collapsed objects is much debated and it is strongly dependent on the local density regime. In particular, as pointed out by Susa (2007), the ignition timing of the source star is crucial in collapsing clouds. If the ignition takes place when the central density is larger than $\sim 10^2$ cm$^{-3}$, the collapse cannot be halted by radiation. However, at the present time, it is still not possible to follow in great detail the formation of the stellar core and the ignition of nuclear reactions that lead to the birth of a star.

As a consequence, cosmological simulations are inevitably affected by resolution issues, mostly at large densities, which limit our understanding of how the various physical processes interplay in the very final stages of star formation. This also affects our abilities to quantify photon escape from the dense star-forming regions. It is reasonable to think that in realistic conditions the inner cores will be optically thick, and that only after the photons have heated up the cloud and thermalized with it will they be able to escape and dissociate molecules in the diffuse IGM. However, there are still no definitive answers on this topics. Furthermore, these many uncertainties can even lead to differences of several orders of magnitudes when comparing the mass estimates of haloes affected by radiation (e.g. Ciardi et al. 2000b; Kitayama et al. 2001; Dijkstra et al. 2004).

5 SUMMARY AND CONCLUSIONS

Cosmic gas and star-forming processes are fundamental in the study of modern astrophysics. However, they are very complicated to

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Figure 9. Evolution of the mean and maximum H$_2$, HD, H$^-$ and H$_2^+$ fractions with redshift for the simulation with (right) and without (left) ionizing radiation. When star formation sets in at redshift $z \sim 11$, the H$_2$ fractions drop fast, where both the mean and the maximum values are affected. The mean HD fraction remains constant in the presence of ionizing radiation and increases with lower redshift in the absence of radiation. The maximum follows the same trend, with the difference that it drops as the first photons begin to propagate. There is only a small change in the evolution of the H$^-$ fraction. Finally, the H$_2^+$ fraction is slightly suppressed from the ionizing radiation.

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If we consider that primordial haloes have radii of a few kpc, the fraction of volume that is interesting for such events is very small. For a protogalaxy having a radius of several kpc and developing a dense core within $\sim 100$ pc, the volume fraction of high-density, possibly shielded, gas is $\lesssim 10^{-3}$.
It is crucial to consider all the involved physical and chemical mechanisms. In the case of early structure formation, primordial chemistry has to be taken into account, because it is mainly via H- derived molecules that the first objects can aggregate gas and form stars. Furthermore, it is also necessary to self-consistently include the RT of the photons produced by stellar sources. Indeed, these travel into the cosmic medium and they can ionize the surrounding gas or dissociate formed molecules. As the impacts of RT on the chemical evolution of the early Universe are expected to be significant, it is important to couple such calculations in order to obtain a reliable picture.

In this paper, we have presented numerical methods of coupled chemistry treatment and multifrequency RT, applied to N-body, hydrodynamical simulations. We have used the SPH code GADGET-3, which is an extended version of the publicly available code GADGET-2 (Springel 2005). We have also included the RT implementation of Petkova & Springel (2009) and the non-equilibrium chemistry implementation of Maio et al. (2007), following e−, H, H+, H2, He, He+, He++, H2+, H2++, D, D+, HD and HeH+.

After a detailed description of the coupling between the RT treatment (Section 2.1) and the non-equilibrium chemical treatment (Section 2.2), we have performed convergence tests (Section 3) and cosmological applications (Section 4) of our code.

We have started (Section 3.1) with the expansion of an ionized sphere around a stellar-type source emitting at a temperature of $\sim 3 \times 10^4$ K in a uniform-density gas. We have traced the element and molecular evolution with time and we have compared the analytical results (in Figs 2 and 3). We have found that analytical analyses based on H-only gas at a constant temperature give a sufficient criterion to predict the evolution of the I-front.

The different species reach different ionization radii. We have used the Strömgren radius, defined for H-only gas at $10^8$ K, as a reference. Deuterium species recombine at a radius comparable (within 10 per cent) to the Strömgren radius, while He becomes completely neutral at $\sim 2/5$ of the Strömgren radius. H$_2$ has an ionization radius that is typically larger than the Strömgren radius, by about 40 per cent ($\sim 7$ kpc versus $\sim 5$ kpc). The compression of gas because of the propagating I-front enhances molecular species (H$_2$ and HD) in the outer layers, where temperatures are around $\sim 10^2$–$10^3$ K. The high values of the creation rates in these temperature regimes also make H$_2$ and HD increase by a few orders of magnitude.

The second test (see Section 3.2) is a mean-density cosmological evolution, where the CMB was assumed to be the only source of ionizing radiation. We found that, because of the low cosmic background emission, the CMB does not significantly affect the abundance evolution, even when considering photon propagation at very high redshift (Fig. 6).

As applications of the numerical methods have previously been described, we have studied (Section 4) the effects of RT on the chemical evolution of primordial gas (e.g. Fig. 7). We have performed cosmological simulations of structure formation with and without ionizing radiation from stellar sources, and we have checked the consequences for molecular formation and destruction.

We have found that the presence of ionizing radiation from stars depletes molecular hydrogen up to several orders of magnitude (see Fig. 8), by inhibiting the main formation paths (the H$^-$ channel and the H$_2^-$ channel) and by dissociating it via LW radiation. Our results are consistent with those of other authors (e.g. Johnson et al. 2007; Wise & Abel 2007; Ahn et al. 2009; Trenti & Stiavelli 2009; Whalen et al. 2010; Latif et al. 2011), who studied the impacts of the UV background in destroying the H$_2$ molecule. In addition, we have found that other molecules that also form in pristine gas, such as HD, are strongly suppressed by radiative feedback (Fig. 9).

There are large discrepancies in the quantitative assessments of the impacts of radiative feedback on baryonic structure formation in the current literature. In fact, different authors (e.g. Ciardi et al. 2000b; Dijkstra et al. 2004) have shown uncertainties of several orders of magnitudes on the basic estimates of the masses of the haloes affected by radiation. Such determinations could even be highly biased by their different post-processing approaches. Indeed, in order to have large statistics or to circumvent numerical complications, these authors do not consider hydrodynamics self-consistently coupled with RT and non-equilibrium chemistry. This could be problematic for coming to reliable conclusions, because, as shown by our numerical simulations (Section 4), the RT effects on gas evolution could be quite important and they could affect star-forming regions in a non-negligible way. The destruction of early molecules by stellar sources has a large effect on the following star formation processes, because it hinders the successive birth of metal-free stars. This also implies the need for different viable low-temperature coolants, such as metals (e.g. Maio et al. 2007), or the presence of ionized gas (Yoshida et al. 2007), to sustain star formation at later times.

Thus, the obvious expectation is that the popIII star formation rate will drop (even more heavily than expected by Tornatore et al. 2007; O’Shea & Norman 2008; Hasegawa et al. 2009; Maio et al. 2010, 2011a; Johnson & Kochfar 2011), and that the popII contribution will easily dominate the lower-redshift Universe.

However, further and more detailed investigations of high-resolution numerical simulations are required in order to draw final and definitive conclusions on this topic.

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