Reionization scenarios and the temperature of the intergalactic medium

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ABSTRACT

We examine the temperature structure of the intergalactic medium (IGM) due to the passage of individual ionization fronts using a radiative transfer (RT) code coupled to a particle-mesh N-body code. Multiple simulations were performed with different spectra of ionizing radiation: a power law (\(\propto \nu^{-0.5}\)), miniquasar, starburst, and a time-varying spectrum that evolves from a starburst spectrum to a power law. The RT is sufficiently resolved in time and space to correctly model both the ionization state and the temperature across the ionization front. We find that the post-ionization temperature of the reionized IGM is sensitive to the spectrum of the source of ionizing radiation, which may be used to place strong constraints on the nature of the sources of reionization. RT effects also produce large fluctuations in the He II to H I number density ratio \(\eta\). The spread in values is smaller than measured, except for the time-varying spectrum. For this case, the spread evolves as the spectral nature of the ionizing background changes. Large values for \(\eta\) are found in partially ionized He II as the power-law spectrum begins to dominate the starburst, suggesting that the large \(\eta\) values measured may be indicating the onset of the He II reionization epoch.

Key words: radiative transfer – methods: N-body simulations – methods: numerical – diffuse radiation – large-scale structure of Universe.

1 INTRODUCTION

The process by which the Universe was reionized is one of the premier unsolved questions in cosmology. Measurements of the Ly\(\alpha\) optical depth of the intergalactic medium (IGM) along quasi-stellar object (QSO) lines of sight (LOSs) require the IGM to have been reionized by \(z \gtrsim 6\) (Becker et al. 2001), consistent with recent measurements of the cosmic microwave background (CMB) by the Wilkinson Microwave Anisotropy Probe (WMAP), although a higher redshift of \(z \sim 11\) is preferred, with a 2\(\sigma\) upper limit of \(z \lesssim 17\) (Spergel et al. 2007). The sources of the reionization are currently unknown. The most recent estimates of the numbers of high-redshift QSOs suggest that QSOs are too few to have ionized H I prior to \(z \approx 4\), without an upturn in the QSO luminosity function at the faint end (Meiksin 2005). While an adequate supply of ionizing photons is likely produced within young, star-forming galaxies, it has yet to be conclusively demonstrated that the ionizing photons are able to escape in sufficient numbers to meet the requirements for reionization (Fernández-Soto, Lanzetta & Chen 2003; Malkan, Webb & Konopacky 2003). Other, more speculative, possibilities include pockets of Population III stars (e.g. in young galaxies or star clusters, Choudhury & Ferrara 2006) or miniquasars (Madau et al. 2004).

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the dominant ionizing sources on the temperature of the post-ionized IGM, considering both soft sources like galaxies and hard sources like QSOs. Rather than performing a full reionization simulation with multiple sources, which is still beyond the current resources of numerical computations, we limit the computations to a single I-front sweeping across the box, as would occur prior to the time of the complete overlap of I-fronts. Although this approximation will not allow us to compute precise values for the ionization fractions of hydrogen and helium for comparison with measurements, as these levels will be reset by the subsequent total photoionization rates after I-fronts overlap, it does permit a quantitative evaluation of the temperature structure after complete reionization. This is because, once ionized, the temperature is insensitive to the total intensity or shape of the ionizing background (Meiksin 1994; Hui & Gnedin 1997), which will readjust both due to the overlapping of I-fronts and due to the evolution of the sources and photoelectric optical depth of the IGM.

The simulations are performed with an RT code coupled to an N-body code to model the evolution of the IGM. In Section 2, the algorithm and the numerical code are described. The details of the simulation volume and sources are given in Section 3. Results of the simulations are provided in Section 4 and discussed in Section 5.

## 2 Method

The simulation code, PMRT_MPI, is the merger of a Lagrangian particle-mesh (PM) code (Meiksin, White & Peacock 1999), and a grid-based RT code which are modularly independent. We perform the RT on the evolving gas density field, as computed by the PM code. Full hydrodynamical simulations have shown that the gas density closely traces the dark matter density down to the Jeans scale (∼100 kpc) (Cen et al. 1994; Zhang et al. 1998). Statistical comparisons between the resulting Lyα forest properties show good agreement at the 10 per cent level (Meiksin & White 2001; Viel et al. 2002).

The gas density is taken as a constant fraction (Ω_b/Ω_m) of the total density. This is a fair approximation since baryons trace dark matter (Zhang et al. 1998) and in simulations with gas, the gas to total density. This is a fair approximation since baryons trace dark matter down to the Jeans scale (∼100 kpc) (Cen et al. 1994; Zhang et al. 1998). Statistical comparisons between the resulting Lyα forest properties show good agreement at the 10 per cent level (Meiksin & White 2001; Viel et al. 2002).

The I-fronts propagate much faster than the sound speed, so that the pressure-response of the gas has only a small effect on the reionization. The PM code evolves the density field assuming that all mass is collisionless, interacting only gravitationally.

The density field is determined from the particle distribution by gridding the particles on to a mesh. To avoid low-count artefacts in low-density regions while not sacrificing information in dense regions, the density field is separated into two fields, ρ(r) = ρ_0(r) + ρ_m(r), and the low-density field, ρ_m(r), is convolved with a Gaussian of radius two grid cells. A threshold cell count (N_{mesh} = 5 for these simulations) discriminates ρ_m(r) from ρ_0(r). In dense regions, ρ_m(r) = N_{mesh} and ρ_0(r) = ρ(r) - N_{mesh}, while in low-density regions, ρ_m(r) = ρ(r). The smoothed field is then ρ′(r) = ρ_0(r) ⊘ g(r) + ρ_m(r) where g is the Gaussian smoothing kernel.

### 2.1 Radiative transfer

The RT code uses a probabilistic method which is based on the photon-conserving algorithm of Abel et al. (1999), extended to include helium by Bolton et al. (2004) who applied the RT algorithm to a density field frozen in the comoving frame. For convenience, we provide details of the RT code here.

The rates of change in the ionization-state populations due to ionizations and recombinations are given by

\[
\begin{align*}
\dot{n}_{\text{H}1} &= n_i n_{\text{H}1} \alpha_{\text{H}1} - n_{\text{H}1} \Gamma_{\text{H}1}, \\
\dot{n}_{\text{H}2} &= -n_{\text{H}1}, \\
\dot{n}_{\text{He}1} &= n_i n_{\text{He}1} \alpha_{\text{He}1} - n_{\text{He}1} \Gamma_{\text{He}1}, \\
\dot{n}_{\text{He}2} &= -n_{\text{He}1} - n_{\text{He}2}, \\
\dot{n}_{\text{He}3} &= n_{\text{He}2} \Gamma_{\text{He}1} - n_{\text{He}3} \alpha_{\text{He}3}.
\end{align*}
\]

where \( \alpha_i \) is the recombination coefficient from species \( i \) and \( \Gamma_i \) is the photoionization rate. Number-density changes, \( \dot{n}_i \), due to cosmological evolution are accounted for by carrying only the ionization fractions \( f_{\text{HI}} = n_{\text{H}1}/n_i \) and similar for helium fraction \( f_{\text{He}1}, f_{\text{He}2}, \) and \( f_{\text{He}3} \) between PM iterations.

The forms for the recombination coefficients \( \alpha_{\text{H}1}(T) \) and \( \alpha_{\text{He}1}(T) \) are derived from the generalised hydrogenic case A form given in Seaton (1959). For \( \alpha_{\text{He}1}(T) \), the radiative term is from Vernier & Ferland (1996) while the dielectronic term is adopted from Aldrovandi & Pequignot (1973). The recombination coefficients are provided in Table 1.

The photoionization rate per particle, \( \Gamma \), for each species, is dependent on the local mean intensity of radiation, \( J_\nu \), and the ionization cross-section, \( \sigma \), for the species and is given by

\[
\Gamma = 4\pi \int_{\nu_T}^{\infty} \frac{J_\nu}{h\nu} \sigma_\nu \mathrm{d}\nu,
\]

where \( \nu_T \) is the threshold frequency for ionization, which differs for each species. In the plane wave approximation used here, the local

| \( \alpha_{\text{H}1} \) | \( 2.065 \times 10^{-11} T^{-1/2} \left( 6.414 - \frac{1}{2} \ln T + 8.68 \times 10^{-3} T^{1/3} \right) \) |
| \( \alpha_{\text{He}1} \) | \( 3.294 \times 10^{-17} \left( \frac{T}{10^5} \right)^{1/2} \left( 1 + \left( \frac{T}{10^5} \right)^{1/2} \right)^{0.309} \left( 1 + \left( \frac{T}{3.065 \times 10^5} \right)^{1/2} \right)^{1.061} \right)^{-1} + 1.9 \times 10^{-9} \left( 1 + 0.3 e^{-\frac{\nu_T - 15000}{2000}} \right) e^{\frac{\nu_T - 15000}{T^{-3/2}}} |
| \( \alpha_{\text{He}2} \) | \( 8.260 \times 10^{-17} T^{-1/2} \left( 7.107 - \frac{1}{2} \ln T + 5.47 \times 10^{-3} T^{1/3} \right) \) |
| \( \beta_{\text{H}1} \) | \( 2.851 \times 10^{-40} T^{3/2} \left( 5.914 - \frac{1}{2} \ln T + 0.01184 T^{1/2} \right) \) |
| \( \beta_{\text{He}1} \) | \( 1.55 \times 10^{-39} \left( 0.3647 + 1.24 \times 10^{-26} \left( 1 + 0.3 e^{-\frac{T - 15000}{2000}} \right) e^{\frac{T - 15000}{T^{-3/2}}} \right) \times 10^{-39} T^{-1/2} \) |
| \( \beta_{\text{He}2} \) | \( 1.140 \times 10^{-39} T^{1/2} \left( 6.607 - \frac{1}{2} \ln T + 7.459 \times 10^{-3} T^{1/3} \right) \) |
Table 2. Ionization cross-section parameters used in equation (6).

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_T (\text{m}^2)$</th>
<th>$n_T (\text{Hz})$</th>
<th>$\beta$</th>
<th>$s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{\text{H}i}$</td>
<td>$6.30 \times 10^{-22}$</td>
<td>$3.282 \times 10^{15}$</td>
<td>1.34</td>
<td>2.99</td>
</tr>
<tr>
<td>$\sigma_{\text{He}i}$</td>
<td>$7.83 \times 10^{-22}$</td>
<td>$5.933 \times 10^{15}$</td>
<td>1.66</td>
<td>2.05</td>
</tr>
<tr>
<td>$\sigma_{\text{He}ii}$</td>
<td>$1.58 \times 10^{-22}$</td>
<td>$1.313 \times 10^{16}$</td>
<td>1.34</td>
<td>2.99</td>
</tr>
</tbody>
</table>

mean intensity is simply the radiation field incident on the volume attenuated by the cumulative optical depth,

$$4\pi J_\nu = \frac{L_\nu}{4\pi r_0^2} e^{-\tau_\nu},$$

where $L_\nu$ is the luminosity of the source per frequency, $r_0$ is the distance of the source from the volume, and $\tau_\nu$ is the cumulative optical depth which, at a distance $R$ from the source, is

$$\tau_\nu(R) = \sigma_T n_{\text{H}i} + \sigma_T n_{\text{He}i} + \sigma_T n_{\text{He}ii}.$$  

(4)

where the cumulative column depth from the edge of the box to $R$ is

$$N_i(R) = \int_{r_0}^{R} n_i(r) \, dr.$$  

(5)

The ionization cross-sections are approximated using the form given in Osterbrock (1989):

$$\sigma(\nu) = \sigma_T \left[ \beta \left( \frac{\nu}{\nu_T} \right)^{-2} + (1 - \beta) \left( \frac{\nu}{\nu_T} \right)^{-4} \right].$$  

(6)

The parameters for the various species are listed in Table 2. The reionization is further restricted by imposing a check on the position of the light front to ensure that gas is not ionized too early. Neglecting this effect can lead to an overestimate of the temperature (Madau, Meiksin & Rees 1997).

The equations governing the thermal state of the gas are used in their entropic form. The entropy is parametrized by the function

$$S = \frac{P}{\rho \gamma},$$  

(7)

where $P$ is the pressure, $\rho$ is the gas density, and $\gamma = 5/3$ is the adiabatic index for a monatomic gas. It follows from equation (7) that

$$S = (\gamma - 1)\rho^{-\gamma}(G - L),$$  

(8)

where $G$ and $L$ are the thermal gain and loss functions per volume, and

$$T = \frac{\mu m_e}{k} S \rho^{\gamma-1},$$  

(9)

where $\mu$ is the mean molecular weight of the gas, $m_e$ is an atomic mass unit, and $k$ is the Boltzmann constant.

Heating is provided by the excess energy above the ionization threshold $h\nu_T$ of the ionizing photons. For a single species of density $n_i$,

$$G = 4\pi n_i \int_{\nu_T}^{\infty} \frac{J_\nu}{\nu} (\nu - \nu_T) \, d\nu.$$  

(10)

Since all species contribute, the total heating rate is

$$G = G_{\text{H}i} + G_{\text{He}i} + G_{\text{He}ii}.$$  

(11)

Cooling is provided by recombinations, collisional excitation of the excited levels in neutral hydrogen, and inverse-Compton scattering of CMB photons. As for heating, all species contribute to cooling, giving the total cooling rate

$$L = L_{\text{H}i} + L_{\text{He}i} + L_{\text{He}ii} + L_{\text{C}}.$$  

(12)

For a single species, recombinations radiate the electron energy $\sim kT$ as photons at the rate $L_i = n_i n_e\beta_i(T)$. For $\text{H}i$ and $\text{He}ii$, the recombination cooling coefficients $\beta_i(T)$ are, as $\alpha_i(T)$, from Seaton (1959). For the $\text{He}i$ radiative term we use the expression in Black (1981) while we combine the approximation $\beta_{\text{He}i} = 3 \, \text{R} \, \alpha_{\text{He}i}$ (Gould & Thakur 1970) with the second $\alpha_{\text{He}i}$ term listed in Table 1 for the dielectronic component (Aldrovandi & Pequignot 1973). The total recombination cooling coefficients are provided in Table 1.

For the cooling rate from collisional excitation of $\text{H}i$ we adopt the approximation of Spitzer (1978):

$$L_{\text{C}} = \frac{4\pi d \sigma_T}{m_e} n_e T_{\text{CMB}}(z) [T - T_{\text{CMB}}(z)].$$  

(14)

where $\sigma_T$ is the Thomson cross-section, $a$ is the radiation energy density constant, $m_e$ is the electron mass, $c$ is the speed of light, and $T_{\text{CMB}}$ is the temperature of the microwave background.

In the current implementation, the simulations do not solve for the overlapping of I-fronts. Rather, they describe the passage of the first I-front across a neutral region. Reionization will also be affected by the hydrodynamical response of the gas, which is not included here. For low to moderately overdense systems, this has only a moderate effect on the statistical properties of the resulting absorption systems (Meiksin & White 2001). The hydrodynamical effects are more important for reionization in denser structures like minihaloes, which can be optically thick at the Lyman edge. Ionization heating results in an overpressure that drives the gas out of the minihaloes, reducing their densities and making them less effective at slowing the I-fronts. Estimates based on the photon consumption rate suggest that the role of these systems in slowing the fronts is small (Ciardi et al. 2006).

Another simplification is the absence of diffuse radiation. Radiative recombinations produce a diffuse radiation field throughout the ionized region. Besides the recombination rate, the intensity depends on the amount of clumping of the gas. Estimates range from a boost in the ionization rate by an additional 10–40 per cent. (Meiksin & Madau 1993; Haardt & Madau 1996). After the gas has been ionized, the diffuse field may be accounted for by rescaling the overall radiation level, as the intensity of the radiation field has a negligible effect on the post-ionization gas temperature. Radiative recombinations will also contribute to the reionization process itself. The contribution, however, is generally negligible for both hydrogen and helium reionization (Shapiro & Giroux 1987; Miralda-Escude & Ostriker 1990; Meiksin & Madau 1993; Madau & Meiksin 1994). An exception is in dense regions in a scenario in which the $\text{He}ii$ I-front precedes the $\text{H}i$ I-front. In this case, assuming that all photons produced by helium recombinations to the ground state of $\text{He}ii$ are locally absorbed by neutral hydrogen atoms, the time to ionize $\text{H}i$ is

$$t_{\text{He}ii-H} \approx \frac{n_{\text{H}i}}{S n_{\text{He}i} \sigma_{\text{He}ii}^{\text{re}}} \approx 7.7 \times 10^{20} \left( \frac{\Omega_{\text{b}} h^2}{0.020} \right)^{-1} \frac{T_4}{1 + \delta (1 + z)^{-3}}.$$  

(15)

where $\sigma_{\text{He}ii}^{\text{re}}$ is the radiative recombination rate to the ground state of $\text{He}ii$, $T_4$ is the gas temperature in units of $10^4$ K, and $\delta$ is the local
fractional overdensity. An allowance has also been made for 1.5 additional secondary electrons produced per photoionization (Shull 1979). Compared with a Hubble time of $t_{\text{Hubble}} \approx 14$ Gyr $(1 + z)^{-3/2}$, the ionization time goes as

$$\frac{t_{\text{He II}}}{t_{\text{Hubble}}} \approx 640 T_4^{2.5} \frac{1}{(1 + z)^{3/2}(1 + \delta)}.$$  

(16)

For the range of source turn-on redshifts considered ($8 < z < 20$), except in very overdense regions, this ratio will be large and hydrogen will remain largely neutral in the interval between helium and hydrogen ionization. The effect on the temperature will therefore be small, except for very overdense regions. After reionization, the post-ionization temperature will be accurately computed even in the highly overdense regions since the temperature is set by the balance between ionization heating and radiative cooling with no memory of the reionization history retained (Meiksin 1994).

Heating by X-rays is automatically included, but not the effect of secondary electrons. The secondary electrons have a negligible effect on the post-ionization temperature of the gas (Madau et al. 1997). Ahead of the I-front, however, the heating rates will be overestimated by a factor of 2–5, depending on optical depth to the ionizing photons (which determines their mean energies) (Shull & van Steenberg 1985). While the tendency to approach thermal equilibrium reduces the impact of the secondaries on the ionizing photons (which determines their mean energies) (Shull & van Steenberg 1985), the post-ionization temperature will be accurately computed even in the highly overdense regions since the temperature is set by the balance between ionization heating and radiative cooling with no memory of the reionization history retained (Meiksin 1994).

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None of the above simplifications affects our findings presented in this paper, which concentrates on the post-ionization thermodynamic properties of the IGM as it relates to the Ly$\alpha$ forest.

2.2 Implementation

To solve the RT equations, we use the probabilistic formulation described in Abel et al. (1999), as extended to multiple species by Bolton et al. (2004). In the probabilistic formulation, the ionization rate per unit volume due to an incident photon flux per frequency interval, $F_\nu$, is given by

$$n \Gamma = \frac{1}{D} \int_{0}^{\infty} F_\nu \sigma_{i,\nu} n \, d\nu,$$

(17)

and approximated as

$$n \Gamma = \frac{1}{D} \int_{0}^{\infty} F_\nu \left(1 - e^{-\tau_{\text{cell}}^\nu} \right) \, d\nu,$$

(18)

where $\tau_{\text{cell}}^\nu = \sigma_{i,\nu} n \, d\nu$ is the optical depth of a single cell of width $d\nu$. This formulation conserves photons and does not lead to excessive ionizations through cells for which $\tau_{\text{cell}}^\nu > 1$. For multiple species, the probability of absorption is spread among the various species and the rate of ionization must be known for each species. Bolton et al. (2004) describes the split for absorption by H I, He I, and He II. Using their shorthand $p^i = e^{-\tau^i}$ and $q^i = 1 - e^{-\tau^i}$ where the values of $\tau^i$ are within the cell (as opposed to cumulative), the probabilities of absorption by each species are

$$p_{\text{abs}}^{\text{He II}} = \frac{q^{\text{He II}} p^{\text{He II}}}{D},$$

(20)

and

$$p_{\text{abs}}^{\text{H I}} = \frac{q^{\text{H I}} p^{\text{H I}} p^{\text{He II}} (1 - e^{-\tau_{\text{cell}}})}{D},$$

(21)

with $D = q^{\text{H I}} p^{\text{H I}} p^{\text{He II}} + q^{\text{He II}} p^{\text{He II}} + q^{\text{He I}} p^{\text{He I}}$ and $\tau_{\text{cell}}^\nu = \tau_{\text{cell}}^\text{H I} + \tau_{\text{cell}}^\text{He II} + \tau_{\text{cell}}^\text{He I}$. Equation (17) with $\sigma_{i,\nu} n \, d\nu$ replaced by the values of $P_{\text{abs}}$ above is the form implemented in PMRTMPI. We recast equation (10) for each species in a similar manner to prevent excessive heating.

Both the PM and RT modules were coded in C and parallelized using a message-passing interface (MPI) (the PM component previously so (see Meiksin et al. 1999)). MPI is suited to work on distributed memory systems, but works equally well on shared memory systems, albeit not with optimal memory use. The RT module consumes most of the processing time. In the RT module, each LOS is processed by a single computer processor element (PE). In general, the time spent by each process on an LOS scales linearly with the resolution along the LOS. In regions of high optical depth, refinements are generated which split the cell into low-optical-depth sections. The number of refinements is a factor in the PE load for an LOS. Load imbalance is possible because the time to process an LOS varies for each LOS, depending on the amount of structure. Load imbalance is alleviated by dynamic (first-come-first-served) allocation of LOSs to processes. The master node performs the allocation and, consequently, has a significantly lower mean load. The load imbalance with the master node can be reduced by either (1) having one physical processor unit execute both the master and a slave process or (2) using many processor units, so that instead of one of few being underused, one of many is underused and less time is spent in a non-load-balanced state.

In addition to accurate modelling of the I-front, special attention is given to computing accurate post-photoionization temperatures. This requires sufficient resolution in time and space to correctly model both the ionization structure of the I-front and the temperature across it. This is particularly important when modelling reionization by sources with hard photons like QSOs. The time-step for the RT is computed, independent of the PM time-step, from the cooling, ionization, recombination, and density-change time-scales. The minimum of these time-scales is multiplied by a factor of 0.2, found through convergence tests using a uniform medium containing He III and H II fronts. Convergence is considered established if the maximum error in the temperature along the LOS (compared with a fiducial run using a factor of 0.1) is less than half a per cent. High spatial resolution at the front is guaranteed by the use of refinements. Any cell in an LOS which is optically thick at the Lyman edge ($\tau > 1$) is split into a sufficient number of slices such that $\tau \leq 1$ in each. Convergence tests were similarly used to establish this criterion by comparing with a fiducial run with $\tau \leq 0.05$ per slice. Refinements are normally only generated at the I-front.

Integration over frequency of the ionization (equation 2) and heating (equation 10) functions is performed using Gauss–Legendre quadrature over the intervals $\nu_{\text{H II}}$, $\nu_{\text{He II}}$, and $\nu_{\text{He I}}$, to $\nu_{\text{He I}}$, to $\nu_{\text{He II}}$, and Gauss–Laguerre quadrature for the interval $\nu_{\text{He II}} \rightarrow \infty$ where $\nu_i$ is the ionization threshold for a species $i$. The integration parameters for each of these intervals were tailored to each of the input spectra using convergence tests similar to those described in the previous paragraph.

Of course, the effort required to get the temperatures correct comes at the expense of computer cycles. More than 20 000 PE hours were required for the simulations presented here. PMRT_MPI
was run in parallel on eight or 16 PEs drawn from a dedicated cluster of IBM OpenPower 720s or a local cluster of LINUX boxes of mixed type.

Validation of the code was accomplished by the use of problems with known solutions and comparison with results produced by an independent code. The analytic solution to the position of a hydrogen I-front in a gas of uniform density irradiated by a monochromatic source with photon energy $h\nu = 13.6$ eV (producing no heating) is easily derivable (e.g. Iliev et al. 2006). We simulated the passage of an I-front through a gas with $n_H = 10^{-3}$ cm$^{-3}$ and $T = 10^4$ K ionized by a source producing photons at a rate of $5 \times 10^{48}$ s$^{-1}$ (test 1 of Iliev et al. 2006). Over a period of 500 Myr (a few times the recombination time-scale), the error in the position of the front was never more than 6 per cent. There is no analytical solution for the gas temperature if irradiated by a non-monochromatic source. However, other simulations exist to which we could compare. One of us (AM) has an RT code which implements an altogether different method with more physics than we included in PMRT\_MPI (Madau et al. 1997). For an $\alpha = 0.5$ power-law spectrum ionizing a uniform IGM at the mean baryon density, this code (with the effect of secondary electrons switched off) produces post-ionization gas temperatures of about 18,000 to 20,000 K at $z = 7$. Including the effect of secondary electrons was found to reduce the post-ionization temperature by about 200 K while the temperature in the gas ahead of the I-front, where helium ionization releases large numbers of electrons, was reduced by about 1000 K. Our PMRT\_MPI code produces post-ionization gas temperatures of 16,000 to 23,000 K at this epoch. PMRT\_MPI generates the correct ionization structure and temperatures that agree with both expectations from observations and the result of an independent code. We are confident that given the physics included, the PMRT\_MPI code is producing correct results.

3 SIMULATIONS

We use PMRT\_MPI to simulate the passage of an I-front produced by sources with a variety of characteristic spectra. Each I-front computed may be considered to result from a single source with the adopted spectrum, or a group of several neighbouring sources with individual I-fronts that have already overlapped, producing a single advancing I-front through the IGM. Because we treat each LOS separately, the resulting temperature distributions may also be considered as produced by distinct sources, and the resulting temperature statistics an ensemble average over the IGM.

In the following, we describe the sources of ionizing radiation (Section 3.1), estimate the expected characteristic scales of their I-fronts at the reionization epoch (Section 3.2), describe the volume of space simulated (Section 3.3) and demonstrate that the results have converged with resolution and are not dominated by cosmic variance (Section 3.4).

3.1 Sources

The source spectra (Fig. 1) were selected to emulate candidate reionization sources. For the power law, the luminosity is given by $L(\nu) \propto \nu^{-\alpha}$ where $\alpha = 0.5$, which corresponds to a hard quasar/QSO/AGN spectrum. The miniquasar spectrum of Madau et al. (2004) is given by $L(x) \propto x^{1.14} + 8x^{-1}$, $1 \leq x \leq 20$; $P(x) \propto 8x^{-1}$, $x \geq 20$ where $x \equiv \nu/\nu_0$. The starburst spectrum was produced by PEGASE\(^1\) (Fioc & Rocca-Volmerange 1997) for a galaxy 30 Myr after a burst of Pop III (zero metallicity) star formation. The starburst spectrum has an effective spectral index of $\alpha_{eff} = 7.4$ just above the Lyman edge. The hybrid model begins with a starburst spectrum, and between $z = 5$ and 4 evolves into an $\alpha = 0.5$ power law, mimicking a radiation field in which a QSO source dominates.

The order of propagation of the H I and He II I-fronts is different for the different sources. For a time-invariant spectrum, the He II I-front precedes the H I I-front if the spectrum is hard enough, specifically if $\alpha_{eff} < 1.8$. The condition is met for both the power-law and miniquasar spectra and, indeed, the He II was ionized prior to H I in those simulations. The starburst spectrum certainly fails the condition as it has negligible intensity above $\nu_{HeII}$. The hybrid spectrum, in which a spectrum dominated by starbursts evolves into one dominated by a power law, leads to the H II I-front preceding that of He II.

To ensure comparable results, all spectra were normalized to produce an incident hydrogen ionizing flux of $1.5 \times 10^7 (1 + z)^2$ s$^{-1}$ m$^{-2}$. This corresponds to a typical flux level driving an I-front, as detailed in Section 3.2. For example, it corresponds to an $L(\nu_{HeII}) = 1.5 \times 10^{21}$ W Hz$^{-1}$ QSO source with $\alpha = 0.5$ at a comoving distance of 5 Mpc. The flux is adequate to ionize the full simulation volume by $z = 3$. We fix the incident flux level to a common level to ensure that differences in the post-reionization temperature are due to the differences in the incident spectra rather than the time-scale for reionization. We also explore the effect of source turn-on redshift by performing, for each source, simulations with the source turning on at redshifts of $z_{on} = 8, 12, 20$. These were selected to cover the range of redshifts limited by WMAP and QSO observations. Because of the common incident flux normalization, these do not correspond to different reionization scenarios in which the reionization of the Universe completes at different epochs, as the reionization histories are nearly identical for $z < 8$. It is simply a device that allows us to ensure the results at late times are insensitive to the assumed turn-on redshift of the sources.

The ionizing radiation is projected as parallel rays normal to the surface of the simulation volume. This configuration has the computational advantage of allowing all radiative calculations for a given ray to be done in a single column, independent of neighbouring columns. Since no information about the thermal state of the gas is carried with the particles as they move from one cell to another.

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\(^1\) http://www2.iap.fr/users/fioc/PEGASE.html.
to complete reionization. We adopt an estimate for the emissivity
be estimated from the total emissivity of all the sources just prior
characteristic luminosity per source, the source space density may
the sources is the inverse of the characteristic volume of the ionized
depth up to $z$ (Meiksin & White 2003, 2004; Meiksin 2005). At
present day value of the Hubble parameter). For a source producing
$z$ gas at the time of overlap is then $N_e = 4.8 \times 10^{29}, 1.0 \times 10^{25}$
and $0.17 \times 10^{55} s^{-1}$, respectively. Allowing for an escape fraction
fraction, equation (22) gives for the characteristic comoving I-front ra-
dius at the time of overlap $R_I \approx 15(f_{esc}/0.1)^{1/3} \text{Mpc}$ for $a_S \approx 2 - 7.4$
(Meiksin 2005). The uncertainty in the ionizing photon conversion
rate and escape fraction corresponds to an additional factor of un-
certainty of about 2 in the size. Addressing the size of the ionized
bubbles in which QSOs reside prior to turn-on, Alvarez & Abel
(2007) show that galaxies ionized regions of the order of tens of
comoving Mpc shortly before overlap.

It is possible that the IGM was reionized by even rarer, more
massive and more luminous systems, such as massive post-starburst
galaxies (Panagia et al. 2005). Allowing for Population III stars and
a high escape fraction, typical I-fronts at the time of overlap could
approach comoving radii of $\sim 30-50$ Mpc.

3.2.2 Active galactic nuclei

The number counts of luminous QSOs fall short of the amount
required to reionize the IGM (Yan & Windhorst 2004; Meiksin
2005). Low-luminosity AGN, however, are plausible sources of non-
stellar ionizing radiation (Ricotti & Ostriker 2004). A population of
galaxies harbouring $10^6 \text{ M}_\odot$ black holes shining at their Eddington
luminosities would require a space density of $n_H \sim 2 \times 10^{-4} \text{Mpc}^{-3}$
to reionize the IGM by $z = 6$ (Meiksin 2005). The corresponding
characteristic comoving I-front radius at the reionization epoch
is then $R_I \approx n_H^{1/3} \approx 17$ Mpc, comparable to that expected for Lyman
break galaxies.

It is likely that the sources that ionized He II to He III were QSOs,
as few other objects produce an adequate supply of sufficiently hard
photons. If the QSOs were low-luminosity QSOs, as above, then the
above estimate for the He II fronts would apply to the He III ionizing
fronts as well. If the rarer luminous QSOs dominated the reion-
ization of He II, the characteristic I-fronts at the time of overlap
would be even larger. For a comoving space density at $3 < z < 5$
of $10^{-7} - 10^{-8} \text{Mpc}^{-3}$ (Meiksin 2005), the characteristic comoving
sizes would be 100–200 Mpc.
3.2.3 Other sources

It is possible that more common structures ionized the IGM, such as collapsed systems smaller than Lyman break galaxies which merged into larger systems. In the simulations of Gnedin (2000), reionization is dominated by systems with total stellar masses exceeding $3 \times 10^{10} M_\odot$. As only a few such systems are responsible for ionizing the gas in a $4 h^{-1}$ Mpc comoving volume, the characteristic I-front size at overlap is a few comoving Mpc. Our models are just marginally applicable to such sources, but more relevant to the rarer larger I-fronts that would occur prior to overlap than the smaller ionized regions.

In the miniquasar model of Kuhlen & Madau (2005), an individual source does not ionize hydrogen much beyond a comoving distance of 20 kpc. In this case, the characteristic I-fronts are much smaller than those we model. Our miniquasar source spectrum corresponds to luminosities much larger than those considered by Kuhlen & Madau (2005). Nevertheless, we adopt the miniquasar model as a physically motivated alternative hard spectral shape. As we show later, the results are nearly indistinguishable from the pure power-law case.

A more exotic source of ionizing radiation is some form of decaying particle. Various hypotheses have been suggested. Our results are not relevant to a scenario in which such particles were responsible for the reionization of the IGM, as the sources are completely localized and ubiquitous.

3.3 Simulation volume

All simulations were performed in a $(25 h^{-1} \text{ Mpc})^3$ comoving volume. This is large enough to include the typical pre-overlap I-front for the models discussed in Section 3.2. A $\Lambda$CDM model was assumed (Spergel et al. 2003), with parameters: $h = 0.71$, $\omega_b h^2 = 0.022$, $\omega_c = 0.268$, $\omega_\Lambda = 0.732$, where $\omega_b$, $\omega_c$, and $\omega_\Lambda$ have their usual meanings as the contributions to $\Omega$ from the gas, all matter and the vacuum energy, respectively. For the hydrogen fraction by mass, $Y = 0.235$.

The initial density perturbations were created by displacing a uniform grid using the Zel'dovich approximation. The initial power spectrum of the density fields was a COBE-normalized power law with index $n = 0.97$. The same initial conditions were used for all simulations, except for the convergence and cosmic variance tests. Since there is no feedback from the RT to the PM code, all the runs have identical gas densities. The simulations were evolved to a redshift of 3.

3.4 Cosmic variance, convergence

The results are subject to cosmic variance and bias from the resolution of the $N$-body code and the RT grid, but not substantially. In this section we describe two extra simulations which ascertain the effects of cosmic variance and a change in the resolution parameters by comparing these with the PLO8 run which they most closely match. We use the $\rho-T$ and temperature distributions (Fig. 2, top and bottom panels) to illustrate the effects. The extra simulations also show that the lack of advection in the simulations is not a source of significant error.

There are two parameters that control the spatial resolution of the simulation: the number of particles in the PM simulation, $N_p$, and the mesh size of the gas density grid, $N_g$. To estimate the variation due simply to cosmic variance, a simulation was run with a different realization of the initial density fluctuations at the same resolution as the main body of runs ($N_p = 256^3, N_g = 256$). In Fig. 2, the difference between the solid (black) and dot–dashed lines (red) indicates the cosmic variance. A simulation with eight times the mass resolution ($N_p = 512^3$) and twice the RT mesh resolution ($N_g = 512$) produced a qualitatively equivalent distribution (Fig. 2, dashed line), bracketed by the two lower resolution realizations.

The current code does not advect thermodynamic quantities. Hence, if a dense halo has a high velocity, the gas in the halo is not properly modelled. The error from the lack of advection is not easy to quantify, but it is not believed to be large. The error is more prominent when cells are smaller since moving gas is more likely to cross a smaller cell. The comparison of the $256^3$ runs to the higher-resolution $512^3$ run (Fig. 2) demonstrates little variation.

4 SIMULATION RESULTS

The simulations provide information for two epochs of interest: the period during which the gas is being ionized and the post-ionization epoch. Our primary focus in this paper is the post-ionization temperature of the gas, but future telescopes such as the Low Frequency Array\(^3\) (LOFAR), the Mileura Widefield Array\(^4\) (MWA), and the main body of runs ($N_p = 256^3, N_g = 256$). In Fig. 2, the difference between the solid (black) and dot–dashed lines (red) indicates the cosmic variance. A simulation with eight times the mass resolution ($N_p = 512^3$) and twice the RT mesh resolution ($N_g = 512$) produced a qualitatively equivalent distribution (Fig. 2, dashed line), bracketed by the two lower resolution realizations.

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\(^3\) http://www.lofar.org.

eventually the Square Kilometre Array\textsuperscript{5} (SKA), will be able to probe the epoch of ionization itself via the red shifted 21-cm line of neutral hydrogen (see Furlanetto, Oh & Briggs 2006, for a review). The reionization epoch will be the topic of a future paper.

In this section, we focus on the thermal state of the gas as established by the passage of an individual I-front. The reionization process involves the overlap of such fronts. The ionization fractions of the gas after the reionization epoch will be constantly reset as the gas sees ionizing photons from an increasing number of sources, both because of the time needed for photons to reach the gas and as new sources turn on (while older ones die). These effects are not accounted for by our single I-front models. The temperature of the gas, however, is nearly insensitive to the continual resetting of the level and shape of the ionizing photon background (Meiksin 1994; Hui & Gnedin 1997). It is instead determined by the reionization process itself and the subsequent evolution of the physical state of the IGM. We here explore the evolution of IGM temperature as computed in our simulations. A principal goal is to determine if the temperature of the ionized IGM is dependent on the nature of the ionizing source. We find that it is, and in Section 4.3 we quantify and discuss the magnitude of this effect and some of its consequences for the ionization structure of the IGM.

The simulation results also permit us to explore a few other issues related to the reionization of the IGM. Clumping of the gas will generally impede the propagation of I-fronts. We evaluate the importance of this effect in Section 4.2. Because of the inclusion of helium ionization in our simulations, we are able to examine the ratio of He\textsc{ii} and He\textsc{iii} to H\textsc{i} in the ionized IGM prior to the epoch of complete He\textsc{ii} reionization. We discuss these results in Section 4.5.

However first, to justify the effort put into the implementation of RT in our code, we make a comparison with the optically thin approximation (OTA) in Section 4.1.

4.1 Comparison with the OTA

Neglecting RT can underestimate temperatures by a factor of a few (Abel & Haehnelt 1999; Bolton et al. 2004; Bolton & Haehnelt 2007). The importance of including RT effects during reionization to obtain accurate temperatures is best illustrated by comparing against a simulation using the OTA. Simply put, the OTA means to self-shield the incoming I-front by dense structures because of the role in hardening the spectrum of the radiation field.

The approximation works fairly well because any gas dense enough to self-shield is also dense enough to reach thermal balance. So the post-ionization temperature is essentially insensitive to the details of reionization. The approximation fails, however, to properly treat low-density gas, because the time to reach thermal equilibrium in low-density gas exceeds the Hubble time at high redshifts. As a consequence, the low-density gas retains a memory of the reionization details. This is particularly important when low-density gas is shielded from the oncoming I-front by dense structures because of their role in hardening the spectrum of the radiation field.

To compare our results with those using the OTA, we performed a simulation in which the cumulative optical depth to any point was set to zero, mimicking the OTA. The $\rho - T$ and temperature distributions for the PL08 model with and without the approximation are illustrated in Fig. 3. Overall the distributions are similar. Since different regions are exposed to different spectra without the OTA, there is more spread than when the OTA is used. The hardening of the spectrum due to selective absorption of low-energy photons heats the gas, particularly in the less dense regions. A high density spur of decreasing temperature with increasing density is produced in both simulations, resulting from the establishment of thermal balance between photoionization heating and atomic cooling (Meiksin 1994).

4.2 Clumping

It has long been recognized that clumping of the IGM gas may substantially slow the propagation of I-fronts due to the increased rate of radiative recombinations (Shapiro & Giroux 1987; Meiksin & Madau 1993; Madau & Meiksin 1994). Estimates of the importance of clumping have varied, but recently tend towards only a moderate slowdown of the I-fronts (Sokasian et al. 2003; Meiksin 2005; Ciardi et al. 2006) with the resistance increasing with time as clumping increases (Iliev, Scannapieco & Shapiro 2005). In our simulations, the slowing of the I-fronts in individual LOSs leads to shadows in the ionization maps, as shown in Fig. 4.

We have estimated the role clumping may play in delaying reionization by comparing the growth of the H\textsc{ii} filling factor in the simulations with that predicted for a uniform IGM at the mean baryon density up to $z = 6$, at which point overlapping I-fronts would completely the reionization. Introducing structure into the IGM actually results in a moderate increase in the rate at which the filling factor of ionized gas grows in the early stages, as shown in Fig. 5. This is because most of the volume of the Universe is underdense. Once half of the volume is reionized, the filling factor converges to the uniform density prediction, with a small slowdown depending on the spectral shape of the source. The evolution of the mass-weighted

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3.pdf}
\caption{Effects of the OTA. The top panels illustrate the $\rho - T$ distribution without (left-hand panel) and using (right-hand panel) the OTA. The lower panels show the modification to the volume-weighted (left-hand panel) and mass-weighted (right-hand panel) temperature distributions produced without (solid line) and with (dot-dashed line) the approximation. The volume-weighted distribution is affected more because most of the volume of the Universe contains underdense regions, which retain a memory of the reionization process.
\end{figure}

Reionization and the temperature of the IGM

Figure 4. The H I fraction at \( z = 6 \). From the top left-hand to bottom right-hand side, the panels correspond to PL20, MQ20, SB20 and HY20. (The hard source has not yet turned on in the hybrid model, so the simulation at this point is identical to the starburst run.) The ionizing flux is incident from the left-hand side. Distances are in proper units.

Figure 5. Fraction of the simulation volume reionized for three models, compared with the case for a uniform density IGM at the mean density. The hybrid model follows the same history as the starburst model prior to \( z = 6 \). A simple model in which a uniform density gas (\( \rho = \Omega_b \rho_c (1 + z)^3 \)) is ionized by a constant flux of ionizing photons is plotted as the solid line. There are three separate redshifts at which the ionizing flux is turned on. All the models initially ionize the gas faster than the uniform density case as the I-front sweeps into underdense regions. Clumping eventually slows down the growth of the H II filling factor by an amount depending on the spectral shape.

4.3 Temperature

Fig. 6 is a map of the temperature distribution at a redshift of \( z = 6 \). Fig. 7 shows a similar map for the power-law model at \( z = 3 \). In both maps, only regions in which the H I was ionized (\( f_{\text{H I}} < 0.1 \)) at \( z = 6 \) are shown. (The remaining gas would have been ionized by a different I-front or fronts by this time.) We immediately see a variety of effects that will be explored quantitatively later. First, the gas temperature in the miniquasar model is virtually identical to that of the simple \( \alpha = 0.5 \) power law. Secondly, the starburst model produces the coolest ionized gas. (At this stage, the hybrid and pure starburst models are identical.) Thirdly, the highest temperatures are typically found just behind the H II I-front. Fourthly, a fraction of ionized hydrogen follows a similar trend including the more rapid rise than the uniform density case at early times. By \( z = 6 \), however, the fraction grows substantially less rapidly, with 50 per cent to a factor of 2 less mass ionized than for the uniform density prediction. The slower growth for the mass-weighted case versus the volume filling factor is expected since it takes longer for the I-front to penetrate the densest regions which contain proportionally more mass.

It is possible the amount by which the I-front slows down is underestimated because of the deficit of small dense structures like Lyman limit systems in N-body simulations (Gardner et al. 1997; Meiksin & White 2004). A definitive result may need to await hydrodynamical simulations that reproduce the statistics of Lyman Limit Systems and denser intergalactic structures.
Figure 6. The temperature at $z = 6$. From the top left-hand to bottom right-hand side, the panels correspond to PL20, MQ20, SB20 and HY20. (The hard source has not yet turned on in the hybrid model, so the simulation at this point is identical to the starburst run.) The ionizing flux is incident from the left-hand side. Only regions for which $f_{HI} < 0.1$ are shown. The remaining gas (masked as blue) would be ionized by other sources.

Figure 7. Density distribution (left-hand panel) and temperature map at $z = 3$. The temperature map is from PL20. Only regions for which the gas is ionized prior to $z = 6$ are shown; the remaining regions are masked as blue.

‘streaking’ effect is apparent. The gas temperature downstream of a dense clump of gas is enhanced compared with the surrounding gas as a result of delayed ionization. The enhancement persists until $z = 3$. Finally, when compared with the gas density, all the models produce gas temperature structure that traces the large-scale gas structure, as illustrated in Fig. 7. The relation, however, is not one of simple proportionality, as we will see below. For instance, because the most recently ionized gas tends to be hotter at a given density, the temperature tends to increase towards the right-hand side (because the I-front passes from the left- to right-hand side), as shown in Fig. 6.

The gas temperatures distinguish the various models at all redshifts. The temperature distributions of the gas ionized by $z = 6$, both volume-weighted (Fig. 8) and mass-weighted (Fig. 9), show clear differences for the different model spectra. At $z = 3$, for the power-law and miniquasar models, the temperatures span $8 - 28 \times 10^3$ K (90 per cent of the gas mass with 5 per cent below the range and 5 per cent above) with a mass-weighted mean of $15 \times 10^3$ K. The hybrid model has a hotter tail in its distribution, ranging from $\sim 10$ to $31 \times 10^3$ K with a mass-weighted mean of $17 \times 10^3$ K. Gas two to three times cooler is produced by the starburst model. For this model, the temperatures at $z = 3$ range from 2000 to 17 000 K.
Reionization and the temperature of the IGM

There are few direct determinations of the IGM gas temperature. The measured Doppler parameters on their own provide only an indication of the spread of the $\rho/T$ coefficients and not an indication of the spread of the $\rho$ distribution. If metal lines are present, however, the thermal and kinematic contributions are separable. By simultaneously fitting CIV and SiIV absorbers, Rauch et al. (1996) found average temperatures of $\sim 38000 \text{ K}$ for systems with $\log_{10} N_{\text{HI}} > 14$. Only the hybrid model is able to achieve temperatures of $T \approx 40000 \text{ K}$ (Figs 8 and 9).

We have tested that the redshift at which the source turns on is not a significant factor. Except for a slight shift to higher temperatures for the $z_{\text{on}} = 8$ models, the curves are nearly identical. This is because the incident ionizing flux has been normalized to a common value for all the cases so that by $z \lesssim 8$ the reionization proceeds in a nearly identical manner. Changing the epoch of reionization would change the temperature in the low-density gas at later times. This effect is not explored here.

As we showed above, the use of full RT instead of an OTA not only further heats the gas, but it also spreads the $\rho-T$ distribution away from a tight power law (Fig. 3). The spread in temperatures is greatest for gas with $\rho/\bar{\rho} > 1$. The spectrum of the ionizing radiation is modified by preferential absorption of the lower frequency photons as they pass through the gas. The modification hardens any spectrum, but is most influential to spectra that already have a hard component. Hence, the spread should be largest for harder spectra.

Fig. 10, which maps the $\rho-T$ distribution at $z = 3$ for the ionized gas for PL20, MQ20, SB20 and HY20, confirms the larger spread in the harder spectra. Also confirmed is the similarity of the state of the gas in the models with the power-law and miniquasar spectra.

Pseudo-hydrodynamical models of the IGM usually adopt a polytropic equation of state for the gas. We fit a polytropic relation, $T = T_0 (\rho/\bar{\rho})^{\gamma-1}$, to the $\rho-T$ distributions at $z = 6, 5, 4$ and 3. The results are shown in Table 4. Note that the errors are for the coefficients and not an indication of the spread of the $\rho-T$ distribution, which is not particularly well described as a single polytropic dependence. For comparison, for the OTA run, for which local heating is balanced by local cooling, we find $T_0 = 13780 \pm 40 \text{ K}$ and $\gamma = 1.527 \pm 0.003$ at $z = 3$, with less spread than found when RT is incorporated. Together, these very different simulations imply a local

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Table 4. Fits to the polytropic relation $T = T_0(\rho/\bar{\rho})^{\gamma-1}$ of the gas for which $f_{\text{HI}} < 0.1$ by $z = 6$. The errors are to the fits and not indicative of the distribution in the $\rho-T$ plane.

<table>
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<th>Model</th>
<th>$T_0$ (K)</th>
<th>$\gamma$</th>
<th>$T_{\text{fl}}$ (K)</th>
<th>$\gamma$</th>
<th>$T_{\text{HI}}$ (K)</th>
<th>$\gamma$</th>
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</thead>
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<td>$17900 \pm 100$</td>
<td>$1.29 \pm 0.01$</td>
<td>$16900 \pm 150$</td>
<td>$1.40 \pm 0.01$</td>
<td>$15400 \pm 140$</td>
<td>$1.52 \pm 0.01$</td>
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<tr>
<td>MQ20</td>
<td>$17900 \pm 120$</td>
<td>$1.34 \pm 0.01$</td>
<td>$16950 \pm 170$</td>
<td>$1.44 \pm 0.01$</td>
<td>$15500 \pm 150$</td>
<td>$1.52 \pm 0.01$</td>
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<tr>
<td>SB20</td>
<td>$4200 \pm 130$</td>
<td>$1.44 \pm 0.03$</td>
<td>$4070 \pm 50$</td>
<td>$1.43 \pm 0.01$</td>
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<td>$1.42 \pm 0.01$</td>
<td>$29250 \pm 250$</td>
<td>$1.036 \pm 0.009$</td>
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</tbody>
</table>

The polytropic fits resulting from the simulations may be compared with those of Schaye et al. (2000) to Keck HIRES spectra. These authors find $T_0 \approx 2.2 \pm 0.2 \times 10^5$ K and $\gamma \approx 1.0 \pm 0.1$ at $z \approx 3$, values most consistent with the late He II reionization hybrid model.

### 4.4 Ionization rates

The varying optical depth to ionizing photons results in fluctuations in the ionizing background. The ionization background is parametrized by the ionization rate, $\Gamma$, which is the number of photoionizations per atom per unit time. A tail towards low ionization rates is found, as shown in Fig. 11. The sharp cut-off at the high end corresponds to low optical depth to the source leading to negligible filtering of the source spectrum. Filtering decreases the ionizing photon flux, lowering $\Gamma$.

A tail in the $\Gamma$-distribution is similarly found in the simulations of Maselli & Ferrara (2005), although without the sharp cut-off at the high end. They model a uniform source distribution filtered through the IGM, accounting for the RT of the ionizing photons using a Monte Carlo algorithm. The absence of the sharp upper cut-off in the simulations of Maselli & Ferrara (2005) is consistent with the discreteness effects of their Monte Carlo RT approach. In the presence of a population of randomly distributed local ionization sources, Meiksin & White (2003) show that the sharp cut-off would be replaced by a power-law tail varying as $\Gamma^{-1.25}$.

### 4.5 Helium

The presence of helium alters the temperature of the IGM after reionization by an amount that depends on the reionization scenario. The epoch of helium reionization (ionization of He II to He III) is still unknown. Measurement of the He II Ly$\alpha$ optical depth suggests that it occurred at $z \lesssim 3$ (Zheng et al. 2004; Reimers et al. 2005), which is consistent with the expected epoch of He II reionization by QSO sources with soft spectra (Meiksin 2005). Measurements of the Ly$\alpha$-forest Doppler parameter, $b$, permit an estimate of the IGM temperature. Theuns et al. (2002) and Ricotti, Gnedin & Shull (2000) claim a temperature jump of about a factor of 2–3 at $z \gtrsim 3$. During the reionization process, and prior to its completion, large fluctuations in the He II to H I absorption signatures may be expected, as the He II ionizing metagalactic UV background will show large spatial variations.

We examine the predictions for these fluctuations from our simulations prior to the completion of He II reionization, by which time the He III I-fronts have completely overlapped.
4.5.1 Thermal effects of helium

The highest temperatures are produced by the hybrid model. The high temperatures are directly attributable to the presence of helium. In the hybrid model, the irradiating spectrum undergoes a transition from a starburst to a power-law spectrum between $z = 5$ and 4. As a consequence, the hydrogen I-front precedes the helium I-front. Since the temperature of ionized gas cannot be raised significantly by changing the radiation field, no matter how hard the spectrum (barring extreme cases like a pure X-ray spectrum), without helium the higher power-law spectrum has no effect on the temperature of the gas previously ionized by the starburst spectrum. Gas that has not yet been ionized is heated to higher temperatures than that ionized by the starburst spectrum since more energy, $h(v - v_0)$, is liberated per ionization. In Fig. 12, bottom panel, the differential heating in a hybrid model without helium ($Y = 0$) is illustrated.

The gas ionized prior to the transition to the power-law spectrum remains unaffected by the transition. The gas previously ionized is ionized and heated to higher temperatures. With helium (top panel of Fig. 12) the transition of the spectrum heats all the gas along the LOS. This is not surprising since the ionization of helium introduces additional heating. What is notable is that the gas is heated to higher temperatures than for the case of a power-law spectrum ionizing a completely neutral medium ($\sim 30,000$ K versus $\sim 16,000$ K, see Fig. 8).

A He II I-front passing through H II-dominated gas leads to a larger jump in temperature than an H I front passing through He II-dominated gas. (Note that in both cases, the final state is fully ionized.) The temperature–entropy relation, equation (9), accounts for the differential temperature jumps. In the case of the He II to He III transition in an H II-dominated gas, the mean molecular weight $\mu$ is reduced by only 7 per cent, leaving any gain in entropy to translate into a gain in temperature. In the alternate case of the H I–He I transition in a gas where He II is the dominant helium species, $\mu$ drops by 45 per cent, almost halving the gain in entropy. There is still a net gain in temperature, but it is only about 10 per cent.

The shallow $\rho$–$T$ profile in the hybrid model results from hotter low-density gas compared with the other models (Fig. 10, lower-right panel). The high temperatures following the recent He II reionization are retained in the low-density gas due to the long time for thermal equilibrium to be established in underdense gas (Meiksin 1994).

4.5.2 Correction to the H I abundances at $z < 6$

Prior to overlap of the H I I-fronts at $z \sim 6$, the ionization state of hydrogen is properly modelled by a single source, as we have in our simulation. Equivalently, a single source is sufficient for modelling the helium fractions prior to overlap of the He II I-fronts at $z \sim 3$. However, at $z \lesssim 6$, a single source is insufficient to fix the hydrogen fractions, since once the Universe is reionized a given region becomes exposed to a large number of ionizing sources. In particular, low-density regions once shadowed by Lyman limit systems along the LOS to the source driving an advancing I-front would be swept over by other I-fronts after the reionization epoch.

In order to compare the helium ionization fractions with the hydrogen, we need to remove the effect of the Lyman-edge shadows on the H I from the simulation data. We do so by correcting the H I abundances by setting $\Gamma_{\text{HI}}$ to a uniform value at any given redshift and solving equation (1) for $n_{\text{HI}}$, the static case. Estimates of the expected distribution of $\Gamma_{\text{HI}}$ after the reionization epoch suggest that it is narrowly peaked, especially for $z < 4$ (Meiksin & White 2003). We set $\Gamma_{\text{HI}}$ to the mean value for the unshadowed gas at the given redshift. A negligible change in the temperatures will be generated by an increased ionization rate after other sources are revealed, so that the local temperature produced during the reionization phase will still apply and so sets the value of the radiative recombination coefficient $\alpha_{\text{HI}}$ in equation (1).

The solution to $n_{\text{HI}}$ is still not entirely correct, since the dense Lyman limit systems should contain self-shielded regions which the correction eliminates. The filling factor of the missing self-shielded regions in the corrected version, however, is much less than that of the shadowed low-density regions. We therefore applied the correction to all the H I data at $z < 6$.

4.5.3 Comparison of He II versus H I absorption prior to complete helium reionization

By having two ionization states, both at higher energies than that of H I, helium provides a means of obtaining information about the abundance of high-energy photons. The ratio of the hydrogen and helium column densities is a function of the spectral shape of the ionizing radiation. Coinciding H I and He II absorption features in QSO spectra have been compared by Zheng et al. (2004) and Reimers et al. (2005), who find large fluctuations in the ratio of He II to H I column densities at $z \lesssim 3$. The presence of fluctuations places constraints on helium reionization models. Gleser et al. (2005) find the patchiness requires short QSO lifetimes ($< 10$ Myr) in models which attribute the patchiness to the discreteness of the QSO spatial distribution.

This choice is arbitrary. We could have assigned the expected value at the corresponding redshift, as determined by matching to the measured Ly$\alpha$ effective optical depth (Meiksin & White 2004), but since $\eta$ is proportional to the ratio $\Gamma_{\text{HI}}/\Gamma_{\text{He II}}$, it is anyway fixed only up to an overall rescaling factor.
The He II fraction at $z = 3$. From the top left-hand to bottom right-hand side, the panels correspond to PL20, MQ20, SB20 and HY20. The regions in which hydrogen is not ionized by $z = 6$ are shaded blue.

Bolton et al. (2006) have argued for a model in which the relative number of rare He II-ionizing QSOs compared with abundant He i-ionizing star-forming galaxies sets the spectral hardness. Here, we concentrate on the relative spread of the fluctuations expected behind He II I-fronts prior to their complete overlap, that is, before the epoch of helium reionization has completed. We base the analysis on the simulation results at $z = 3$ (Fig. 13), which is when observations suggest He II reionization was nearing completion. Local sources of He i-ionizing photons could introduce further fluctuations than those we find. Our simulations thus only set a lower limit to the level of fluctuations expected, arising principally from shadowing and attendant fluctuations in the He II ionization rate, during the final stages of He II reionization.

The hardness index $\eta \equiv n_{\text{He}}/n_{\text{H}}$, is a sensitive probe to the shape of the ionizing background. Ionization fraction fluctuations affect the spread in $\eta$ values while the mean value is set by the mean spectral hardness. Here, we concentrate on the relative spread of the fluctuations in $\eta$, as this is independent of the shape of the spectrum. We do refer to definite values for $\eta$ from our simulations rather than arbitrarily rescaling them, but the physical effects we shall describe are not specific to any specific value of $\eta$.

The ionization states of hydrogen and helium are expected to be linearly correlated, but dependent on the hardness of the local radiation field. This follows from radiative equilibrium, for which the rate equations for hydrogen and helium are derivable by setting $n_i = 0$ in equation (1):

\[
\begin{align*}
\dot{n}_{\text{H}} \Gamma_{\text{HI}} & = n_e s_{\text{HI}} \alpha_{\text{HI}} \\
\dot{n}_{\text{He}} \Gamma_{\text{HeII}} & = n_e s_{\text{HeII}} \alpha_{\text{HeII}}.
\end{align*}
\]  

For the highly ionized gas in the simulations, $f_{\text{HI}} \Gamma_{\text{HI}} \simeq n_e \alpha_{\text{HI}}$ and $f_{\text{HeII}} \Gamma_{\text{HeII}} \simeq n_e \alpha_{\text{HeII}}$, giving

\[
\frac{f_{\text{HeII}}}{f_{\text{HI}}} \simeq \frac{\sigma_{\text{HeII}}}{\sigma_{\text{HI}}} \left( \frac{\Gamma_{\text{HeII}}}{\Gamma_{\text{HI}}} \right).
\]  

(24)

The ratio of $f_{\text{HeII}}$ to $f_{\text{HI}}$ is related to $\eta$ through $\eta = (n_{\text{He}}/n_{\text{H}})(f_{\text{HeII}}/f_{\text{HI}})$, where $n_{\text{He}}/n_{\text{H}} \approx 1/13$ ($\Gamma = 0.235$) is the number ratio of helium to hydrogen atoms. Since He II is a hydrogen-like species, the recombination coefficients scale similarly with temperature. Over the range 10 000–20 000 K, $\sigma_{\text{HeII}} \simeq 5.3 \sigma_{\text{HI}}$. Similarly, the photoionization rates also scale but in a more complicated manner dependent on the spectrum (equation 2). The cross-sections for HI and He II can be approximated by using equation (6) with $\beta$ and $s$ the same for hydrogen-like species, $\sigma_{\text{HeII}} = \sigma_{\text{HI}}/4$, and $\nu_{\text{HeII}} = 4\nu_{\text{HI}}$ (Table 2). Taking the radiation field to have the form $J_\nu \propto \nu^{-\alpha}$, the integral in equation (2) gives for the ratio of photoionization rates $\Gamma_{\text{HI}}/\Gamma_{\text{HeII}} = 2^{\alpha+2}$. Combining this result with equation (24) and $\sigma_{\text{HeII}} \simeq 5.3 \sigma_{\text{HI}}$ gives $\eta \simeq 5.3/13 \times 2^{\alpha+2}$.

The values of $\eta$ found in the simulations fluctuate about this estimate. For PL20, for example, the volume-averaged $\langle \eta \rangle_{\text{vol}} = 11$ at $z = 3$. However, the distribution is highly skewed; the mode and 68 percentile range is $3.3^{+3.4}_{-0.5}$. The derived relation predicts $\eta \simeq 3.2$ for $\alpha = 0.5$, in good agreement with the mode. For MQ20, $\langle \eta \rangle_{\text{vol}} = 14$ and, like PL20, the distribution is highly skewed with the mode $3.8^{+4.0}_{-1.1}$. The $\eta$ distribution is insensitive to redshift for the power-law and miniquasar models. In the case of the hybrid model, the evolution of the $\eta$ distribution is complex after the power-law source turns on. For HY20, the evolution of the $\eta$ distribution is illustrated in Fig. 14. As the He II I-front sweeps through the volume, $\eta$ surges...
to $>1000$. At the same time, the competing effect of the hardening spectrum drives the most probable $\eta$ values down. After the source spectrum has completed the transition to a power law, the most probably $\eta$ value settles at the expected value of $\eta \approx 3.2$ while the shadowed regions provide a high-$\eta$ tail.

The fluctuations that produce the high-end tail of the $\eta$ distribution at $z=3$ arise from the attenuation of the source radiation field at the He II ionization threshold. Recall that we have corrected the data to remove $f_{\text{HI}}$ fluctuations, hence softer (larger values of $\alpha$) local ionizing fields are generated by attenuation. Variations in the local density have only a small role as they modify the local gas temperature which varies the approximation $\alpha_{\text{HeII}} \approx 5.3 \alpha_{\text{HI}}$. Fig. 15 illustrates the interplay of effects. The bulk of the gas resides along the $f_{\text{HeII}}/f_{\text{HI}} \approx 5.3 \times 10^{-12}$ locus in the $f_{\text{HeII}} - f_{\text{HI}}$ plane. Attenuation leads to shadows with larger $f_{\text{HeII}}$ fractions, creating parallel loci of constant $f_{\text{HeII}}/f_{\text{HI}}$. The local overdensity sets the value of $f_{\text{HI}}$, as we have set $\Gamma_{\text{HI}}$ to a constant value. Because of the correction to $n_{\text{HI}}$, the effects of self-shielding are not seen in the $\eta$ distribution. Self-shielding would harden the spectrum, generating $\eta$ values below the bulk of the gas. This effect is seen in the uncorrected simulation data in the few regions in which it occurs.

The magnitude of $\eta$ is sensitive to the input source spectra. For instance, choosing $\alpha = 2$ instead of 0.5 for the power-law spectrum would increase $\eta$ by a factor of 8 for the power-law model to values of $\eta > 30$. Boosting the ratio of the contribution of the galaxy to the QSO spectrum in the hybrid model would achieve a similar effect. The relative spread in the fluctuations of $\eta$, however, is independent of any overall shift in the amplitude or shape of the ionizing background for regions in which both hydrogen and helium are ionized. The spread may be a useful diagnostic of the ionization state of the IGM prior to complete He II reionization. Large fluctuations are found for $\eta$ (or, equivalently, in $f_{\text{HeII}}/f_{\text{HI}}$). At $z=3$, $\eta$ is mostly constant, but there is a small fraction with a large range ($\sim 2$ dex). The extent of the range results both from the inhomogeneities in the radiation field and from a wide spread in gas temperatures due to RT, particularly in the low-density gas which gives rise to most of the He II features. The spread is smaller than found by Zheng et al. (2004), who report a range of at least 2.5 dex in $\eta$ at $z \lesssim 3$. This may indicate the presence of local He II-ionizing sources.

Zheng et al. (2004) and Reimers et al. (2005) report some regions with $\eta > 1000$, suggesting these may be regions for which He II is still not ionized to He III. Fig. 16 is a map of $\eta$ for the hybrid model HY20 at $z=4$ compared with a map of the $f_{\text{HeII}}$ fraction. Large $\eta$ values are found to correspond to regions of high He II fractions. The evolution of the $\eta$ distribution for the hybrid model HY20 is illustrated in Fig. 14. At $z \gtrsim 4$, when the power-law source is just taking over from the starburst in magnitude, high excursions are found for $\eta$, with values reaching up to 3000. These high $\eta$ regions are associated with incomplete He II reionization, where $f_{\text{HeII}} \lesssim 1$. Lowering the redshift at which the power-law source overtakes the starburst would lower the redshift at which these high excursions occur to $z \lesssim 3$. These results suggest that Reimers et al. (2005) may have detected the He II reionization epoch.

In their simulations, Maselli & Ferrara (2005) find a higher value of $\eta \sim 250$, but a smaller spread of only a factor of 2–3, not including the low values of $\eta$ associated with self-shielding. As discussed earlier, our single I-front simulations produce an overabundance of shielded H I gas at $z < 6$, which we have eliminated by correcting the $n_{\text{HI}}$ values to a uniform H I photoionization rate. Their higher value of $\eta$ results partially from the soft spectrum adopted from Haardt & Madau (1996) for QSOs with $\alpha = 1.5$ source spectrum.

We parametrize $f_{\text{HI}}$ by the gas density, $f_{\text{HI}} = \alpha (\rho/\bar{\rho})^\beta$, and similarly for $f_{\text{HeII}}$. The best-fitting values are provided in Tables 5 and 6. Cosmic variance leads to errors in $\alpha$ of about 10 per cent and $\beta$ of about 2 per cent. Although the values of $\alpha$ may be readjusted by changing the magnitude of the ionization radiation background, the values of $\beta$ are invariant for a given source spectrum. The close agreement between the values of $\beta$ for $f_{\text{HI}}$, $f_{\text{HeII}}$, and $f_{\text{HeIII}}$ for the respective models reflects the near-linear dependence between the H I and He II ionization fractions, with a weak residual dependence on density (cf. Fig. 15).

The power-law dependence of ionization fraction on density is expected if the shape of the local ionizing spectrum is constant and the density and temperature are related through a power law. The equilibrium rate equation for hydrogen is $n_{\text{HI}} \Gamma_{\text{HI}} = n_{\text{HI}} n_{\text{HeII}} \alpha_{\text{HI}}$. Assuming almost complete ionization, the ionization fraction is

\[ f_{\text{HI}} \simeq \frac{n_{\text{HI}} \alpha_{\text{HI}}}{\Gamma_{\text{HI}}} \]
We recall that the photoionization rate, $\Gamma_{\text{HeII}}$, is a function of the shape of the local ionizing spectrum. Assuming it is constant and that ionization is almost complete, the neutral fraction follows $f_{\text{HeII}} \propto \rho \alpha_{\text{HeII}}$. Over the temperature range of interest, the recombination rate responds to the temperature as $\alpha_{\text{HeII}} \propto T^{-0.68}$. If the density and temperature are related polytropically, $T \propto \rho^{-1}$, then $f_{\text{HeII}} \propto \rho^{1-0.68\gamma-1}$. From our power-law fits in Table 5, the inferred values for $\gamma$ at $z = 3$ are $1.547 \pm 0.001, 1.566 \pm 0.001$ and $1.139 \pm 0.001$ for PL20, MQ20 and HY20, respectively. For HeII, the inferred values at $z = 3$ are $1.554 \pm 0.001, 1.555 \pm 0.001$ and $1.222 \pm 0.001$ PL20, MQ20 and HY20, respectively. The values of $\gamma$ are nearly identical to those found by directly fitting the $\rho-T$ relation in Section 4.3.

5 DISCUSSION AND CONCLUSIONS

We have coupled an RT code based on a probabilistic photon transmission algorithm to a PM N-body code in order to study the sensitivity of the post-ionization temperature of the Intergalactic Medium on source spectrum. We performed multiple simulations with different spectra of ionizing radiation: a power-law ($\propto 10^{-0.5}$), miniquasar, starburst, and a time-varying hybrid spectrum that evolves from a starburst spectrum to a power law.

The power-law and miniquasar spectra produce almost identical temperature distributions, owing to their similar shapes. A greater difference of temperatures is found between the remaining models. The mass-weighted mean gas temperatures at $z = 3$ are 9000 K for the starburst source, 15000 K for the power-law and miniquasar source, and 17000 K for the hybrid models. A larger difference is found between the power-law/miniquasar and hybrid model temperatures from the polytropic fits to temperature and density. A fit to the polytropic relation, $T = T_0(\rho/\bar{\rho})^{\gamma-1}$, gives $T_0 = 14600 \pm 200, 14500 \pm 160, 3515 \pm 11$ and $18600 \pm 100$ and $\gamma = 1.58 \pm 0.01, 1.57 \pm 0.01, 1.553 \pm 0.002$ and $1.134 \pm 0.005$ for the power-law, miniquasar, starburst and hybrid models, respectively, at $z = 3$. The errors are formal fit errors. The highest temperatures are found in the hybrid model at the end of the transition from starburst to power-law spectra ($z \approx 4$), at which time the temperatures span values up to 40000 K, consistent with measurements of C iv and Si iv absorption systems in the Ly$\alpha$ forest (Rauch et al. 1996).
The He\textsc{iii} I-front passing through H\textsc{ii} I-dominated gas leads to a larger jump in temperature than the H\textsc{i} I-front passing through He\textsc{iii} I-dominated gas. Indeed, in the simulations with the power-law spectrum the temperature increase is only about 10 per cent when a trailing H\textsc{i} I-front passes through gas in which helium is fully ionized. The difference is explained by the decrease in the mean molecular weight when H\textsc{i} is ionized. Hence, a significant temperature change will not be produced around a hard source by the passage of an H\textsc{i} I-front, in contrast to a soft source or a region in which hydrogen was fully ionized prior to helium.

The post-ionization temperature of the IGM may be used as a key observable for identifying the nature of the sources of reionization. While moderate to high overdensity gas establishes an equilibrium temperature in which photoionization heating balances atomic radiative cooling processes, the equilibrium time-scale exceeds a Hubble time in lower density regions, those that give rise to optically thin Ly\textalpha absorption systems. In contrast to optically thin reionization models, we find a broad fanning out of the temperature-density relation for underdense regions, with temperatures exceeding $3 \times 10^4$ K for the hybrid model with late He\textsc{ii} reionization. This may help substantially in reconciling the much larger Doppler parameters for the entire IGM and a precise determination of the resulting statistical properties of the Ly\textalpha forest.

We do not address the effect of the epoch of reionization on the evolution of the gas temperature. Much earlier reionization redshifts for the entire IGM will result in much cooler temperatures, primarily due to intense Compton cooling at high redshift. The effect of the reionization epoch on the subsequent IGM temperature has been explored by Ikeuchi & Ostriker (1986), Giroux & Shapiro (1996) and Theuns et al. (2002) without RT. A degeneracy exists between the epoch of reionization and the nature of the sources on the temperature of the IGM. If the epoch of reionization were determined through some other means as, for instance, its detection in the radio by LOFAR or MWA, the subsequent temperature of the IGM, particularly as revealed by the widths of optically thin Ly\textalpha forest absorbers, could then be used to determine the nature of the sources.

Hardening of the spectrum due to passage through structures with high H\textsc{i} column densities produces fluctuations in the $f_{\text{He}\alpha}/f_{\text{H}\alpha}$ ratio in the shadowed regions behind He\textsc{iii} I-fronts prior to complete He\textsc{ii} reionization. A spread is indeed found in the data at $z \lesssim 3$ (Zheng et al. 2004; Reimers et al. 2005). The observed spread of about 2.5 dex, however, exceeds that found in our simulations at $z = 3$ by about a factor of 3. In particular, values of $\eta > 1000$ are reported by Zheng et al. (2004) and Reimers et al. (2005). It may be that local sources are required to reproduce the wider range of observed values. Alternatively, at $z \gtrsim 4$ values up to $\eta \approx 3000$ are found for the hybrid model, when the power-law source begins to dominate the starburst producing partially ionized He\textsc{ii}. Lowering the redshift at which the power-law spectrum dominates the starburst, thus delaying the He\textsc{ii} reionization epoch, would lower the redshift at which large fluctuations in $\eta$ are produced. It may be that Reimers et al. (2005) have detected the epoch of He\textsc{ii} reionization.

Not explored in detail by this paper is the pre-ionization state of the gas which is relevant to future 21 cm detections. To correctly model the gas will require the incorporation of the production of secondary electrons and the diffuse radiation field. The production of the secondary electrons further cools the gas due both to overcoming the ionization potential and to radiative losses from the consequent enhancement of Ly\textalpha collisional excitation (Shull 1979). A copious number of Ly\textalpha photons could be produced in any region where helium is ionized prior to hydrogen. The photons may have important implications for the detection of the 21-cm signature of the IGM, as they can decouple the spin temperature from the CMB (Madau et al. 1997). The Ly\textalpha photons will also be an additional source of pre-heating through recoils, although the amount is likely to be small before the scattering reaches equilibrium (Meiksin 2006). We are currently including both hydrodynamics and the extra radiative physics in more refined models. The addition of hydrodynamics will also eliminate any limitations owing to the absence of advection.

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