

Heating of the Intergalactic Medium by Hydrogen Reionization

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ABSTRACT

During reionization, the intergalactic medium is heated impulsively by supersonic ionization fronts (I-fronts). The peak gas temperatures behind the I-fronts, T_{reion} , are a key uncertainty in models of the thermal history after reionization. Here we use high-resolution radiative transfer simulations to study the parameter space of T_{reion} . We show that T_{reion} is only mildly sensitive to the spectrum of incident radiation over most of the parameter space, with temperatures set primarily by I-front speeds. We also explore what current models of reionization predict for T_{reion} by measuring I-front speeds in cosmological radiative transfer simulations. We find that the post-I-front temperatures evolve toward hotter values as reionization progresses. Temperatures of $T_{\text{reion}} = 17,000 - 22,000$ K are typical during the first half of reionization, but $T_{\text{reion}} = 25,000 - 30,000$ K may be achieved near the end of this process if I-front speeds reach $\sim 10^4$ km/s as found in our simulations. Shorter reionization epochs lead to hotter T_{reion} . We discuss implications for $z > 5$ Ly α forest observations, which potentially include sight lines through hot, recently reionized patches of the Universe. Interpolation tables from our parameter space study are made publicly available, along with a simple fit for the dependence of T_{reion} on the I-front speed.

Keywords: intergalactic medium – dark ages, reionization, first stars – cosmology: theory

1. INTRODUCTION

Nearly all of the hydrogen in the Universe was reionized and heated by the rise of the first galaxies and quasars. Cosmic Microwave Background (CMB) measurements place the midpoint of this process at $z \approx 8 - 9$ (Planck Collaboration et al. 2016), while Ly α forest observations show that it must have been mostly complete by $z = 6$ (McGreer et al. 2015). When combined with other probes such as the visibility of Ly α emitting galaxies and quasar damping wing analyses, these observations suggest that the end of reionization was likely near $z = 6$ (e.g. McQuinn et al. 2007; Ouchi et al. 2010; Stark et al. 2010; Pentericci et al. 2011; Bolton & Haehnelt 2013; Caruana et al. 2014; Taylor & Lidz 2014; Choudhury et al. 2014; Mesinger et al. 2015; Mason et al. 2018;

Mortlock et al. 2011; Bañados et al. 2018; Davies et al. 2018b). Further constraining the timing and duration of reionization would provide insight into the first sources of ionizing radiation in the Universe (see McQuinn 2016 for a recent review).

One path towards constraining reionization is to look for its heating effects on the intergalactic medium (IGM). As ionization fronts (I-fronts) expand supersonically around the first ionizing sources, they impulsively heat the gas to temperatures between 15,000 – 30,000 K (Miralda-Escudé & Rees 1994; Hui & Gnedin 1997; Tittley & Meiksin 2007; Trac et al. 2008; Venkatesan & Benson 2011; McQuinn 2012; Finlator et al. 2018). We shall refer to the temperature achieved by this impulsive heating as the *post-I-front temperature*, denoted by T_{reion} . After the I-front passes, the gas is driven to cooler temperatures over cosmological timescales pri-

marily by the expansion of the Universe and inverse Compton scattering with CMB photons.

The impact of reionization on the thermal history of the IGM is in principle detectable in the small-scale structure of the Ly α forest (e.g. Lidz et al. 2010; Becker et al. 2011; Garzilli et al. 2012; Iršič et al. 2017). The volume-weighted mean temperature rises steadily during reionization, reaches a peak near the end of this process, and declines before the onset of He II reionization (e.g. Upton Sanderbeck et al. 2016; Doussot et al. 2017; Puchwein et al. 2018). The detection of a rise in temperature with redshift at $z > 5$ would be a tell-tale sign of reionization, and would place constraints on its timing and the nature of its sources. It may also be possible to detect spatial variations in the temperature owing to the inhomogeneity of reionization (Trac et al. 2008; Cen et al. 2009; Furlanetto & Oh 2009a; Lidz & Malloy 2014; D'Aloisio et al. 2015; Keating et al. 2018). However, theoretical predictions for both of these signatures are highly uncertain.

Post-I-front temperatures are the chief source of uncertainty for theoretical models of the thermal history. To illustrate this point, Fig. 1 shows the thermal histories of mean-density gas parcels that are impulsively heated to different temperatures. The dashed and solid curves assume $T_{\text{reion}} = 15,000$ and $25,000$ K, respectively, representative of the range of values that are found in the literature (e.g. McQuinn 2012; Puchwein et al. 2018; Finlator et al. 2018). For the post-reionization photoheating rate, we assume a power-law spectrum such that $J_\nu \propto \nu^{-\alpha}$ with $\alpha = 1$ (J_ν is the specific intensity and ν is frequency).¹ Though the effects of T_{reion} are modest for the gas parcels reionized at redshift $z_{\text{re}} = 9$, there are 50 % differences in the $z = 5.5$ temperatures for those reionized at $z_{\text{re}} = 6.5$. Note also that larger T_{reion} leads to larger temperature dispersion, which can be seen from the spread between parcels reionized at $z = 6.5$ and 9. For comparison, the dotted curves adopt $\alpha = 2$ for $T_{\text{reion}} = 25,000$ K, illustrating the effects of uncertainties in the *post-reionization* photoheating rate.² Variations of $\Delta\alpha = 1$ lead to modest $\lesssim 15$ % differences in temperature at $z \sim 5.5$. This simple illustration suggests that T_{reion} plays an important role in interpreting $z > 5$ Ly α forest measurements, which may probe recently reionized patches of the IGM.

¹ In detail, we assume that the spectrum has a sharp cutoff at 4 Ry, which is motivated by models in which stellar emissions dominate the ionizing background at the redshifts of interest (e.g. Faucher-Giguère et al. 2009; Haardt & Madau 2012; Puchwein et al. 2018).

² In §3.1, we will show that $\alpha = 1 - 2$ is within the range of expectation from theoretical models of young stellar populations.

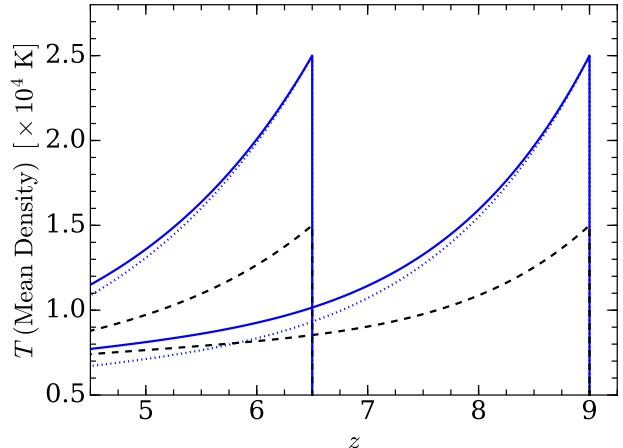


Figure 1. The impact of uncertainties in T_{reion} on IGM temperatures at $z \gtrsim 5$. We model the impulsive heating from a passing I-front by instantaneously heating gas parcels to a temperature T_{reion} . Here we show two illustrative sets of examples in which mean-density parcels are reionized at $z = 6.5$ and 9. We vary T_{reion} from 15,000 (dashed) to 25,000 K (solid), representative of the range of values that have been assumed in the literature. Uncertainties in T_{reion} translate to large uncertainties in the expected temperature of recently reionized gas. For comparison, another significant source of uncertainty in the gas temperature is the post-reionization photoheating rate, which is set by the spectral index of the ionizing background, α . We have assumed $\alpha = 1$, but the dotted curves show the modest effects of assuming $\alpha = 2$ for the case with $T_{\text{reion}} = 25,000$ K.

In principle, it is possible to mitigate these uncertainties because the physics that determines T_{reion} is well known (Miralda-Escudé & Rees 1994). The characteristic width of I-fronts during reionization is several times the mean free path through the neutral gas. The spectrum of incident radiation sets the maximum possible temperature, $3k_B T \sim 13.6 \text{ eV}/(\alpha - 1)$, e.g. $T \sim 50,000$ K for $\alpha = 2$. However, collisionally excited (H I Lyman-series) line cooling by neutrals within the I-front can cool the gas to significantly lower temperatures, depending on how long it spends inside the front. This, in turn, depends on how quickly the I-front is moving, which is set by the number flux of ionizing photons on the front boundary. (As we will show, the actual temperatures are rarely higher than 30,000 K.) In summary, T_{reion} depends mainly on the spectrum of the ionizing radiation and the speeds at which the fronts are moving.

The above discussion highlights why T_{reion} remains so uncertain. First, without observational constraints on the sources and sinks of ionizing photons during reionization, neither the spectrum of the background nor the I-front speeds are known with certainty. Secondly, given the short spatial and time scales associated with the

I-fronts, it is not obvious that cosmological radiative transfer (RT) simulations are converged with respect to T_{reion} . In this paper, we present a focused study that aims to improve our understanding of the T_{reion} parameter space. This study will inform future Ly α forest measurements by making clearer the connection between IGM temperatures and the nature of the reionization process.

Following Miralda-Escudé & Rees (1994), a number of authors have explored T_{reion} (Tittley & Meiksin 2007; Trac et al. 2008; Venkatesan & Benson 2011; McQuinn 2012; Finlator et al. 2018). Some of these studies have reached different conclusions about the likely values of T_{reion} . For example, McQuinn (2012) used 1D RT simulations to argue that post-I-front temperatures should be in the range $T_{\text{reion}} = 20,000 - 30,000$ K. On the other hand, Finlator et al. (2018) examined T_{reion} values in the Technicolor Dawn cosmological RT simulations and found $T_{\text{reion}} = 14,000 - 19,000$ K. In addition to the lack of consensus amongst past studies, the exact dependence of T_{reion} on the incident spectrum and the I-front speed has not been explored in detail. In this paper, we expand upon previous works by performing the first systematic study of the T_{reion} parameter space. For this task, we use a suite of high-resolution, 1D RT simulations to ensure that our results are numerically converged in T_{reion} . After defining the parameter space, we then apply stellar population synthesis modeling, and a set of cosmological RT simulations, to explore what contemporary models of reionization predict for T_{reion} .

The remainder of this paper is organized as follows. In §2, we present our parameter space study of T_{reion} . In §3, we attempt to narrow this parameter space using expectations from current models of ionizing source spectra and I-front speeds during reionization. In §4, we discuss the implications of our results for the thermal history of the IGM and for high- z Ly α forest measurements. We offer concluding remarks in §5. Unless otherwise noted, all distances and velocities are quoted in *physical* units.

2. POST-I-FRONT TEMPERATURES

In this section, we present our parameter space study of T_{reion} . We begin by describing the numerical methodology of our calculations.

2.1. Numerical Methodology

Our calculations are based on the 1D RT code of Davies et al. (2016), which employs the numerical approach of Bolton & Haehnelt (2007). We refer the reader to those papers for technical details. In summary, the code tracks the propagation of ionizing radiation from

a point source into hydrogen and helium gas at a fixed redshift. The 1D RT, ionization balance, and temperature equations are solved on a uniform spatial grid with cell size $\Delta x = 1$ proper kpc. We initialize the gas to a temperature of 100 K, but our results are insensitive to this choice. The gas density is uniform, set to the cosmic mean of the epoch under consideration. (However, in the next section we will explore in a controlled manner the impact of density variations.)

The spectrum of ionizing radiation is discretized over 25 logarithmically spaced frequency bins between 1 and 4 Ry. In Appendix A we demonstrate the numerical convergence of our results with respect to the spatial cell size and frequency binning. We adopt a power-law spectrum characterized by the spectral index α_{IF} , such that the specific intensity of the radiation is $J_\nu \propto \nu^{-\alpha_{\text{IF}}}$, where ν is frequency. The sharp cutoff at energies above 4 Ry is motivated by the standard assumption that stellar sources dominated the ionizing photon budget during reionization (e.g. Shapiro & Giroux 1987; Faucher-Giguère et al. 2009; Haardt & Madau 2012; Becker & Bolton 2013; D’Aloisio et al. 2017). We neglect secondary ionizations, which have an insignificant effect for the adopted source spectrum. The code includes H I, He I, and He II photoheating, and all of the relevant cooling processes for intergalactic gas of primordial composition: collisional excitation, adiabatic expansion, Compton, recombination, free-free, and collisional ionization. The code assumes that the timescale for photoelectrons to thermalize with the neutrals in an I-front is much shorter than the time that the gas spends inside the front. (In fact, to our knowledge, all previous calculations have adopted this assumption.) We justify this assumption in Appendix B.

We have run a suite of RT simulations spanning a range of source luminosities and α_{IF} . We measure I-front speeds (v_{IF}) directly from the simulations by tracking the location of the $x_{\text{HI}} = 0.5$ boundary with time. In a given run, the I-front begins at its fastest speed and slows down with time, since the ionizing flux scales as r^{-2} (where r is the distance from the point source). This allows us to sample a range of v_{IF} within a single simulation, and our runs vary the source luminosities to achieve a wider range of v_{IF} .

As noted above, our primary goal is to quantify how T_{reion} depends on v_{IF} and the spectral index of the ionizing radiation. Two things complicate the use of the aforementioned RT code for this purpose: (1) At a given I-front location, we would like to extract the gas temperature immediately after the I-front has passed to avoid the onset of cooling processes. However, as we consider I-fronts of various speeds and widths, there is no single,

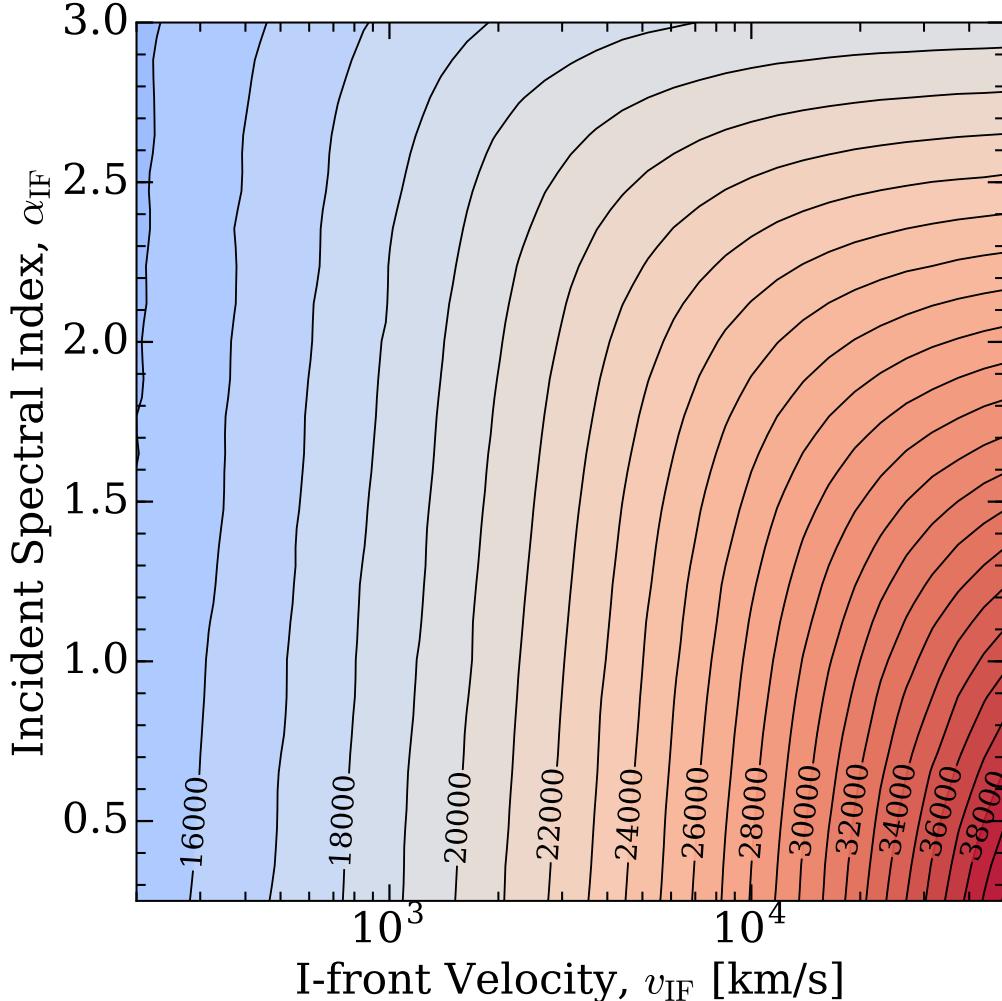


Figure 2. The parameter space of post-I-front temperatures during reionization. The curves show contours of constant T_{reion} in Kelvin. The y -axis corresponds to the spectral index of the incident ionizing radiation, while the x -axis corresponds to the proper I-front speed. The contours are insensitive to redshift and gas density for the bulk of the low-density IGM (see top panel of Fig. 4). In §3, we use stellar population synthesis modeling to argue that spectral indices of $\alpha_{\text{IF}} \lesssim 1.5$ are most relevant during reionization. Using cosmological RT simulations of reionization, we find that the I-fronts are slow during the early stages of reionization, with speeds ranging from $10^2 - 2 \times 10^3$ km/s, but near the end of reionization they reach speeds $\sim 10^4$ km/s.

robust prescription for when T_{reion} should be measured; (2) Absorption by residual neutral gas in equilibrium between the source and the I-front tends to harden the spectrum of radiation impinging on the I-front. The degree of hardening will vary with distance to the source, and with its luminosity. To make the interpretation of T_{reion} unambiguous, we would like to roll these effects into the parameter α_{IF} , such that it is the spectral index of the radiation that is *incident* on the I-front.

We have developed a method of circumventing both of these issues at once. We modified the RT code to turn off Hubble and Compton cooling, as these processes dominate the cooling *after* the gas leaves the I-front, operat-

ing over cosmological time-scales.³ In addition, we turn off all thermal evolution for post-I-front gas that has reached H I ionization equilibrium, i.e. cells for which $(\Delta n_e/n_{\text{tot}})(\Delta x/c/dt) < 10^{-8}$, where Δn_e is the change in the electron number density in time step dt , n_{tot} is the number density of gas particles (atoms, ions, electrons), and c is the speed of light. Importantly, this preserves the relevant heating and cooling processes while the gas is still inside the I-front, but after the I-front passes the temperature remains fixed, allowing us to simply mea-

³ The characteristic time that gas spends inside an I-front is given by equation (B1). For $v_{\text{IF}} = 1,000$ (10,000) km/s (velocities spanning most of reionization; see §3.2), $t_{\text{IF}} \sim 10$ (1) Myr.

sure T_{reion} from the last simulation output. To reduce the effects of spectral hardening, we also set the neutral fraction of this equilibrium gas to an arbitrarily low value. In this limit, the radiation that is incident on the I-front has the same spectral index as that of the source, α_{IF} . From here on we will identify α_{IF} with the incident radiation. We have tested our T_{reion} results against those from the original version of the code, verifying that they are consistent in the regime where spectral hardening is negligible for the latter (see Appendix A).

Lastly, we note that our 1D RT code adopts an infinite speed of light for computational efficiency. Previous studies have shown that this approach provides an exact solution to the I-front propagation along the line of sight to the source. A change of coordinates can be applied to translate the simulation results to the case with finite speed of light (White et al. 2003; Shapiro et al. 2006; Bolton & Haehnelt 2007; Davies et al. 2016). We obtain the true I-front speeds using the velocity correction $v_{\text{IF}} = v_{\text{IF},c=\infty}/(1 + v_{\text{IF},c=\infty}/c)$, where $v_{\text{IF},c=\infty}$ is the speed measured in the simulation. In practice, this correction only comes into play for I-front speeds near the end of reionization.

2.2. Results

Figure 2 shows the main result of this paper: the post-I-front temperature (T_{reion}) as a function of the spectral index of incident radiation (α_{IF}) and I-front speed (v_{IF}). The curves correspond to contours of constant T_{reion} at $z = 6$ and $\Delta = 1$, where Δ is the gas density in units of the cosmic mean. A distinguishing feature of Fig. 2 is that T_{reion} is only mildly sensitive to α_{IF} over much of the parameter space, especially in the hard spectrum limit (small α_{IF}). This behavior is the result of an interplay between the photoheating and the cooling that occurs in the boundary layer of the I-front. Collisional line excitation cooling is exponentially sensitive to temperature and is most efficient when there are equal numbers of neutrals and electrons. Making the spectrum harder increases the energy injection into the gas and broadens the I-front such that there is more collisional line cooling.

To illustrate these effects, Fig. 3 shows the ionization and thermal structures for I-fronts with $\alpha_{\text{IF}} = 2.5$ and 0.5 , and $v_{\text{IF}} \approx 6,000$ km/s. The top panel shows the H I fractions, x_{HI} , where the x -axes have been shifted such that $x_{\text{HI}} = 0.5$ at $R = 50$ kpc. Note that the sharp cutoffs in the top panel owe to our procedure for rolling the effects of spectral hardening into α_{IF} , and the gas temperatures are not allowed to evolve to the left of those cutoffs (as described in §2.1). The bottom and mid-

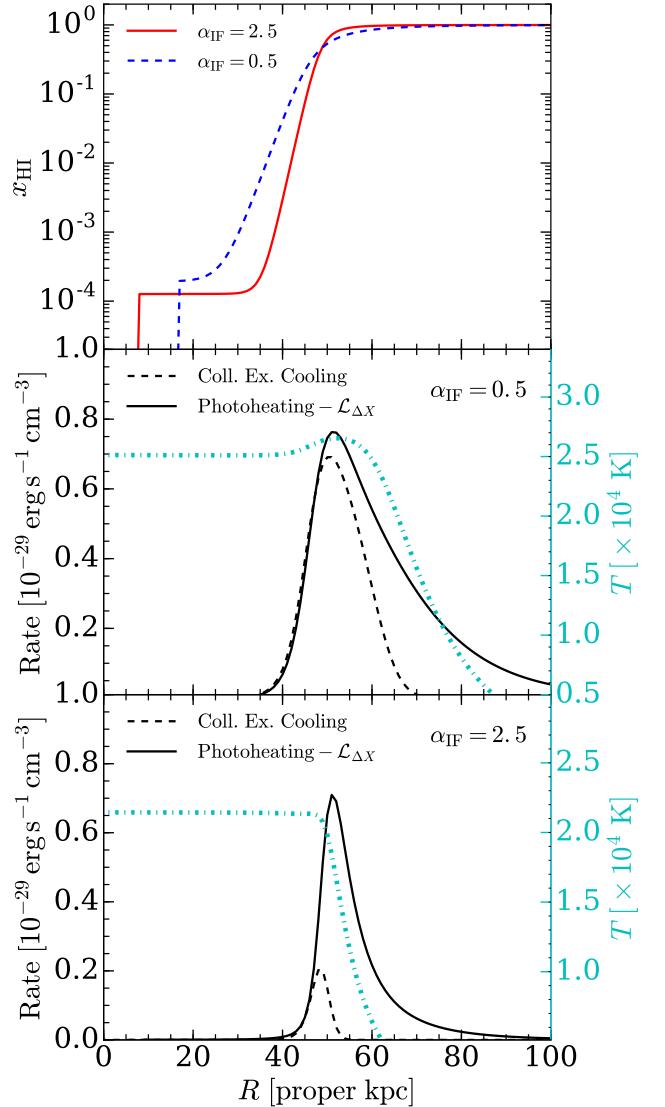


Figure 3. Ionization and thermal structures of I-fronts. Top panel: the H I fraction as a function of distance for two cases illustrating that I-fronts are broader for harder spectra. The solid and dashed lines correspond to $\alpha_{\text{IF}} = 2.5$ and 0.5 , respectively. The x -axes have been shifted such that $x_{\text{HI}} = 0.5$ at $R = 50$ kpc, and both fronts are traveling at $v_{\text{IF}} \approx 6,000$ km/s at $z = 6$. The sharp cutoffs in x_{HI} owe to our methodology for rolling the effects of spectral hardening into the parameter α_{IF} (see §2.1). Middle and bottom panels: the corresponding temperatures (cyan dot-dashed/right-axis), H I + He I photoheating rates (solid) and collisional excitation cooling rates (dashed). (See text for discussion on $\mathcal{L}_{\Delta X}$.) The photoheating from a hard incident spectrum is compensated by the increased collisional excitation cooling rate (owing to its steep dependence on temperature) over a wider area.

dle panels show the corresponding temperatures, as well as H I + He I photoheating and collisional excitation cooling rates. For the former, we have subtracted off $\mathcal{L}_{\Delta X} = (3/2)k_B dn_{\text{tot}}/dt$ (where k_B is Boltzmann's constant), which accounts for the fact that the heat must be distributed amongst nearly twice the particles in the newly ionized gas (see eq. 4). For $\alpha_{\text{IF}} = 0.5$, there is more photoheating over a broader path length. In the absence of cooling, this would result in significantly hotter temperatures compared to the case with $\alpha_{\text{IF}} = 2.5$. However, the steep dependence of the cooling rate on temperature and the wider I-front conspire to keep the increase in T_{reion} modest.

The contours in Fig. 2 are insensitive to redshift over the range of interest for reionization. This property may be understood using a simple scaling argument from Davies et al. (2016), and noting that the main effect of redshift in our homogeneous simulations is to rescale the gas density. Consider an I-front with instantaneous speed v_{IF} . As noted above, the gas in the front would be heated to some maximum temperature determined by α_{IF} in the absence of cooling. However, line cooling will lower the temperature by an amount $\Delta T \sim t_{\text{IF}} L_{\text{cool}} / n_H$, where t_{IF} is the time spent within the front and $L_{\text{cool}} \sim n_H^2$ is the cooling rate. For fixed v_{IF} , the time spent in the front is $t_{\text{IF}} \propto R_{\text{IF}} / v_{\text{IF}} \propto 1/(n_H v_{\text{IF}})$, where R_{IF} is the front width, implying that $\Delta T \propto 1/v_{\text{IF}}$. It follows then that T_{reion} should be insensitive to z at fixed v_{IF} .

The above argument implies that T_{reion} should also be insensitive to Δ as long as the recombination time is much longer than the collisional excitation cooling time. We have explored this dependence numerically by performing a set of RT simulations in which the source luminosity is varied to keep v_{IF} fixed over the range of $\Delta = 0.1 - 10$. The top panel of Fig. 4 shows the results of these runs. The dashed, solid, and dot-dashed curves show the dependence of T_{reion} on Δ for $\alpha_{\text{IF}} = 0.5, 1.5$, and 2.5 , respectively. For these runs, we adopt $z = 6$ and a fixed I-front speed of $v_{\text{IF}} = 9 \times 10^3 \text{ km s}^{-1}$. The blue solid curve corresponds to a slower speed of $v_{\text{IF}} = 9 \times 10^2 \text{ km s}^{-1}$ at $z = 10$ with $\alpha_{\text{IF}} = 1.5$. (In §3.2, we will find that these two speeds are representative of their corresponding redshifts.) The main point is that T_{reion} depends weakly on Δ at fixed v_{IF} , consistent with the simple scaling argument of the last paragraph.

Next we examine the dependence of T_{reion} on the local gas density *for a fixed ionizing flux*. As I-fronts sweep through the IGM, density variations in the cosmic web modulate the local I-front speeds, accelerating through under-densities and slowing within over-densities. Thus, recently reionized gas should exhibit an inverted temperature-density relation with hotter

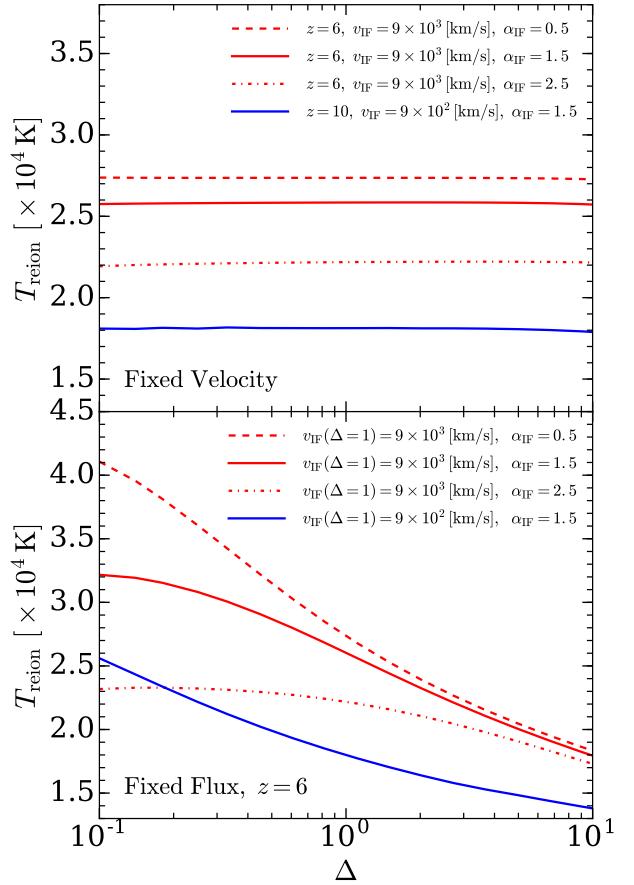


Figure 4. Dependence of post-I-front temperatures on gas density. Top panel: T_{reion} vs. Δ for fixed I-front speed. Post-I-front temperatures are insensitive to the gas density for $\Delta = 0.1 - 10$ at fixed v_{IF} . The top three curves illustrate the effect of varying α_{IF} from $\alpha_{\text{IF}} = 0.5$ to 2.5 . The bottom curve considers a slower front speed at $z = 10$. Bottom panel: T_{reion} vs. Δ for fixed ionizing flux (i.e. the front speed varies with local density). The I-fronts accelerate through (slow down in) regions of under(over)-dense gas, resulting in a hotter (cooler) temperatures. This inverted temperature-density relation is a potential signature of recently reionized gas.

(cooler) temperatures corresponding to under(over)-dense gas. Note that this is not the same as the inversion that owes to gas parcels being reionized at different times. In the latter case, over-dense regions tend to be colder because they are reionized earlier, so they have had more time to cool (see e.g. Trac et al. 2008; Furlanetto & Oh 2009b). In contrast, the inversion under consideration here applies to gas that is reionized at nearly the same time, and owes entirely to the density dependence of I-front speeds. To investigate the magnitude of this effect, we have run a series of RT simulations at fixed ionizing flux spanning a range of Δ at $z = 6$ (near the likely end of reionization). As our primary

motivation is exploring the signature of recently reionized gas in high- z quasar absorption spectra, we neglect shock heating, which is insignificant at the densities considered (McQuinn & Upton Sanderbeck 2016). The bottom panel of Fig. 4 shows the $T_{\text{reion}}-\Delta$ relation derived from our simulations. To connect these results to the contour plot in Fig. 2, we denote these runs by their I-front speeds at $\Delta = 1$. As anticipated, the post-I-front temperature decreases with density, reflecting the fact that I-fronts travel slower through larger Δ . For example, T_{reion} varies by $\approx 5,000$ K between $\Delta = 0.3$ and 3. The trend is stronger (weaker) for harder (softer) spectra.

Based on the results of this section, we are led to conclude that T_{reion} can be determined for most of the intergalactic gas if the local v_{IF} and, to a lesser extent, α_{IF} are specified. Indeed, following the results in Fig. 2, T_{reion} may be determined to within 1000 K for $\alpha_{\text{IF}} \lesssim 1.5$ using the I-front speed alone. We provide a five-parameter polynomial fit to $\ln(T_{\text{reion}})$ at fixed $\alpha_{\text{IF}} = 1.5$,

$$\ln(T_{\text{reion}}) = \sum_{n=0}^4 C_n \ln \left(\frac{v_{\text{IF}}}{[\text{km/s}]} \right)^n, \quad (1)$$

where $(C_0, C_1, C_2, C_3, C_4) = (9.5432, -1.6441 \times 10^{-2}, -9.8010 \times 10^{-3}, 4.1664 \times 10^{-3}, -2.2710 \times 10^{-4})$. We find that eq. (1) is accurate to within 2% over the range $v_{\text{IF}} = 1 \times 10^2 - 7 \times 10^4$ km/s. In §4, we will describe a procedure for using this fit to model the inhomogeneous thermal history of the IGM. For more detailed applications in which the full dependences on α_{IF} and v_{IF} are required, we have made publicly available the numerical data for Fig. 2, as well as a simple code for setting up an interpolation.⁴

3. MODEL EXPECTATIONS

Having established the dependence of T_{reion} on v_{IF} and α_{IF} , we now seek to determine what current models of reionization predict for these quantities. This will allow us to hone in on the expected values of T_{reion} . We begin by considering stellar population synthesis modeling of reionization sources in §3.1. We then quantify v_{IF} from cosmological reionization simulations in §3.2

3.1. Spectra of reionization sources

In what follows, we assume that Population II stars were the primary sources of ionizing photons during reionization. We use the Flexible Stellar Population Synthesis (FSPS) code to model the source spectrum

(Conroy et al. 2009; Conroy & Gunn 2010). Our fiducial calculations correspond to a single, instantaneous burst of star formation with the initial mass function (IMF) of Chabrier (2003), but we have also explored cases using the Salpeter (1955) and Kroupa (2001) IMFs.⁵ We find that our results are insensitive to the choice owing to the fact that they differ mainly at sub-solar stellar masses – a regime which contributes little to the ionizing photon output. On the other hand, choosing a more top-heavy IMF could significantly impact the spectrum as we discuss below. We adopt the MESA Isochrones & Stellar Tracks (MIST; Dotter 2016; Choi et al. 2016; Paxton et al. 2011, 2013, 2015).⁶ For a detailed comparison of the ionizing spectra of MIST to other models, we refer the reader to Choi et al. (2017).

Here we consider the time-integrated spectrum, $\mathcal{S} = \int dt L_\nu(t)$, where $L_\nu(t)$ is the specific luminosity at time t . To perform the integral, we sample $L_\nu(t)$ at 100 logarithmically spaced times between $t = 10^{-4}$ and 500 Myr. We have checked that our results are converged with respect to these choices. Most of the ionizing photons are produced in the first ten million years by massive, short-lived stars. The time-integrated spectrum should provide a reasonable estimate for the average spectral shape that would be incident on I-fronts if reionization were driven by bursty star formation. Below, we will discuss additional effects neglected here that would harden the spectrum.

The red and blue curves in the top panel of Fig. 5 show the integrated spectra for stellar metallicities of $Z = 10^{-3} Z_\odot$ and $Z = 10^{-1} Z_\odot$, respectively, roughly bracketing the range of Z found in simulated $z \gtrsim 6$ galaxies with halo masses $M = 10^9 - 10^{12} M_\odot$ (Ma et al. 2016). The units on the y -axis are arbitrary. (In practice the normalization would be set by the bolometric source luminosity, and our sole focus here is the shape of the spectrum at energies greater than 13.6 eV.) For reference, the dashed curves correspond to power laws with logarithmic slopes $\alpha = 0.5, 1.5$, and 2.5 , where we have anchored these curves on the time-integrated spectra near 13.6 eV.⁷ The bottom panel compares against results from a different isochrone and stellar track model

⁵ We adopt lower and upper IMF limits of $0.08 M_\odot$ and $120 M_\odot$, respectively.

⁶ It was necessary to download additional isochrones because FSPS does not (by default) come with isochrone libraries extending to the lowest metallicities considered here ($Z = 10^{-3} Z_\odot$). See <http://waps.cfa.harvard.edu/MIST>

⁷ Here we use α to distinguish this quantity from the spectral index of radiation that is incident on the I-fronts, α_{IF} , as the latter may be somewhat lower owing to hardening effects neglected here (see last paragraph of §3.1).

⁴ cat.ucr.edu

at $Z = 10^{-1} Z_{\odot}$. For the red curve, we use the PAdova and Trieste Stellar Evolution Code (PARSEC) model (Bressan et al. 2012), which yields a somewhat softer spectrum. This difference owes in part to the effects of stellar rotation, which are modeled in MIST (see Choi et al. 2017).

We can extract *effective* spectral indices by matching the mean excess energy per hydrogen ionization between a power-law model and the FSPS spectra. For the MIST models, we estimate effective indices of $\alpha = 0.9(0.7)$ and $1.9(1.4)$ for $Z = 10^{-3} Z_{\odot}$ and $Z = 10^{-1} Z_{\odot}$, respectively, assuming optically thick (thin) heating. Likewise for PARSEC we obtain $\alpha = 2.3(1.8)$ for $Z = 10^{-1} Z_{\odot}$. More rigorously, we have also performed RT runs using the FSPS spectra (see Appendix A). For the MIST models, we find that the T_{reion} values are consistent with $\alpha \approx 0.9$ and 1.75 for the $Z = 10^{-3}$ and $10^{-1} Z_{\odot}$, respectively. For the PARSEC model we find $\alpha \approx 2.25$ for $Z = 10^{-1}$. These values are much closer to the α that we estimated under the assumption of optically thick heating. Our results indicate that the spectra of metal poor stellar populations are comparable to, or harder than, the spectra of $z = 2$ quasars at energies between 1 and 4 Ry. For example, Lusso et al. (2015) measured $\alpha = 1.70 \pm 0.61$ in this regime from their stack of 53 quasars at $z \approx 2.4$.

There are several reasons to suspect that the (galaxy-sourced) ionizing background during reionization may have been somewhat harder than the estimates given here. First, our calculations neglect the filtering effects of optically thick H I in the ISM of the host galaxy, and within the cosmic web. Absorption by this gas would have hardened the spectrum of the ionizing radiation as it escaped the galaxy and traveled through the IGM (e.g. Madau 1995; Faucher-Giguère et al. 2009; Haardt & Madau 2012). These effects were likely strongest during the last stages of reionization, when the radiation typically had to travel large distances to reach the I-fronts. Secondly, our calculations neglect the effects of binary star systems. Mass transfers and mergers between binary companions can extend the period over which ionizing photons are produced by the stellar population, which would harden the time-integrated spectrum (Eldridge & Stanway 2009; Stanway et al. 2016). Lastly, recent studies have suggested that the IMF in starburst galaxies may be more top-heavy than the IMF assumed here (Baugh et al. 2005; Gunawardhana et al. 2011; Marks et al. 2012; Zhang et al. 2018). Most recently, Schneider et al. (2018) measured a logarithmic slope of $1.90^{+0.37}_{-0.26}$ in the mass range $15 - 200 M_{\odot}$, using spectroscopic measurements of the 30 Doradus star forming region in the Large Magellanic Cloud. (The

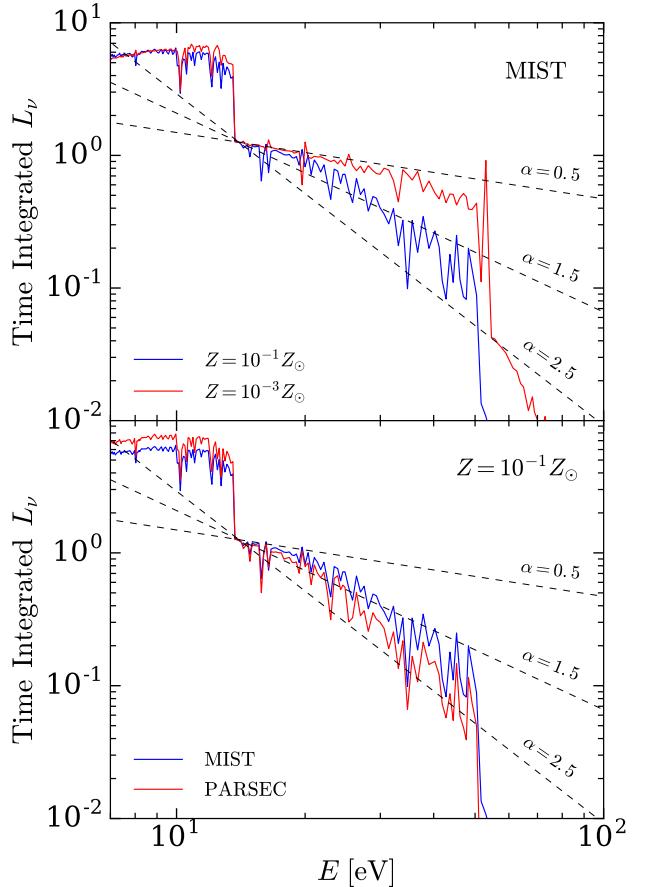


Figure 5. Stellar population synthesis models of time-integrated source spectra during reionization. The units on the y -axis are arbitrary. The top panel shows spectra from our fiducial MIST model with $Z = 10^{-3} Z_{\odot}$ and $Z = 10^{-1} Z_{\odot}$. For reference, the dashed lines correspond to power laws with spectral indices $\alpha = 0.5, 1.5$, and 2.5 . The bottom panel compares against the PARSEC model at $Z = 10^{-1} Z_{\odot}$.

IMF adopted here has a slope of 2.3 for $M > M_{\odot}$, and a cutoff of $120 M_{\odot}$.) Each of the above effects would work in the direction of making α_{IF} smaller. Based on the above considerations, we argue that the lower half of Fig. 2, with $\alpha_{\text{IF}} \lesssim 1.5$, is likely the most relevant region of parameter space for T_{reion} . In what follows, we shall adopt $\alpha_{\text{IF}} = 1.5$ as our fiducial value, but we note that T_{reion} is only mildly sensitive to α_{IF} except at the fastest I-front speeds. In the next section we will find that $v_{\text{IF}} = 10^4$ km/s is close to the upper limit achieved by I-fronts in cosmological simulations, which yields $T_{\text{reion}} = 26,200$ K assuming $\alpha_{\text{IF}} = 1.5$ (see Fig. 2). This result varies by $\Delta T_{\text{reion}} = -4, 200(+1, 600)$ K if we instead assume $\alpha_{\text{IF}} = 2.5(0.5)$.

3.2. I-front speeds during reionization

In this section, we present calculations of I-front speeds in cosmological simulations of reionization.

3.2.1. The SCORCH simulation suite

We extract I-front speeds from the *Simulations and Constructions of the Reionization of Cosmic Hydrogen* (SCORCH) suite (Trac et al. 2015; Price et al. 2016; Doussot et al. 2017). In these simulations, the ionizing sources are populated with an abundance matching scheme that connects the UV luminosity of a source to the mass accretion rate of its host halo (see Trac et al. 2015 for more details). The reionization simulations were run with the RadHydro code (Trac & Pen 2004; Trac & Cen 2007; Trac et al. 2008). The Eulerian hydrodynamics module employs non-equilibrium solvers for the ionization and energy equations, and the RT is carried out with adaptive ray tracing based on the HEALPix formalism (Górski et al. 2005). The radiation spectrum – discretized into five energy bins above 13.6 eV – is derived from the stellar population synthesis modeling of Bruzual & Charlot (2003). To reduce computational costs, the simulations adopt a reduced speed of light approximation in which c_{sim} increases in proportion to the radiation filling factor (i.e. the fraction of cells containing rays), with a minimum value of 0.01c. This prescription yields $c_{\text{sim}}/c \approx 0.2, 0.6$ and 0.9 at volume-weighted ionized fractions of $Q_{\text{HII}} = 0.1, 0.5$ and 0.9, respectively. We note that these values are larger than the minimum values quoted by previous studies for obtaining reliable I-front speeds. For example, Deparis et al. (2018) recently found that $c_{\text{sim}}/c \gtrsim 0.3$ is required to recover I-front speeds reliably throughout reionization, with this condition being relaxed to $c_{\text{sim}}/c \gtrsim 0.05$ during the earliest phases of H II bubble expansion (see also Gnedin 2016).

The SCORCH suite consists of three simulations in an $L_{\text{box}} = 50 h^{-1}\text{Mpc}$ box, with $N_{\text{dm}} = N_{\text{gas}} = 2048^3$ dark matter particles/gas cells, and $N_{\text{rt}} = 512^3$ RT cells. Three different reionization histories were produced by varying the escape fraction of ionizing radiation, which is parametrized by the redshift-dependent form, $f_{\text{esc}} = A_{\text{esc}}[(1+z)/9]^{\beta_{\text{esc}}}$. By design, the simulations all yield a Thomson scattering optical depth of $\tau_{\text{es}} \approx 0.06$, and a reionization midpoint of $z \approx 7.5$. In what follows, we will utilize two of the runs, which we denote using the value adopted for the power-law slope, $\beta_{\text{esc}} = 0$ and 2, with the latter being our fiducial run.⁸ The reionization histories in these runs corre-

⁸ Here we use a different notation than in Doussot et al. (2017). Our β_{esc} parameter corresponds to their a_8 .

spond to the purple and orange curves in Fig. 6 of Doussot et al. (2017), respectively. The end of reionization ($Q_{\text{HII}} = 0.99$) occurs at $z = 6.6(5.6)$ in the $\beta_{\text{esc}} = 0(2)$ run, and the duration of reionization – defined here as the redshift interval between $Q_{\text{HII}} = 0.1$ and 0.99 – is $\Delta z = 3.1(4.8)$. Both of these models are consistent with the latest CMB and Ly α forest constraints on the timing and duration of reionization (McGreer et al. 2015; George et al. 2015; Planck Collaboration et al. 2016).⁹

In addition to the standard hydro and RT data outputs, the code also stores the redshift at which each Eulerian cell is reionized. In practice, this is achieved by recording the earliest redshift at which a cell crosses the 50% ionized threshold. We shall refer to this local quantity as the reionization redshift, z_{re} , which plays a central role in our analysis below.

3.2.2. Methodology

We use two independent methods of extracting I-front speeds from the SCORCH simulations.

Gradient Method: The first method utilizes the reionization redshifts of neighboring cells to compute the local I-front velocity. Consider a cell at comoving coordinate \mathbf{x} that is reionized at redshift $z_{\text{re}} = z$. The proper velocity of the I-front that reionizes the cell can be derived from the local gradient of the z_{re} field,

$$\mathbf{v}_{\text{IF}}(\mathbf{x}) = \frac{a}{|\nabla z_{\text{re}}|} \frac{dz}{dt} \hat{\mathbf{n}} \quad (2)$$

where the derivatives are with respect to the comoving coordinates \mathbf{x} , a is the cosmological scale factor, and $\hat{\mathbf{n}} = (\nabla z_{\text{re}}/|\nabla z_{\text{re}}|)|_z$ is the unit normal vector to the I-front. (We note that this method of estimating I-front speeds is identical to that of Deparis et al. 2018, which appeared on the archive during the preparation of this manuscript.) The z_{re} fields of the SCORCH simulations are saved at the hydro grid resolution of $N_{\text{gas}} = 2048^3$. As a first step, we smooth the field by convolving with the coordinate-space top-hat function, with smoothing length $L_{\text{box}}/N_{\text{rt}} \approx 98 h^{-1}\text{kpc}$ comoving.¹⁰ This is motivated by the fact that the code can only physically track the propagation of I-fronts at the RT resolution. We then apply a four-point finite difference to obtain the gradient, ∇z_{re} .

⁹ We note that the CMB probes the mass-weighted ionized fraction and not, strictly speaking, the volume-weighted quantities quoted here. This distinction is not important given the (still large) uncertainties, however.

¹⁰ Alternatively, we also tried re-binning to the RT grid resolution. We found very similar results between the two methods, with the re-binning method leading to more noise in the v_{IF} fields.

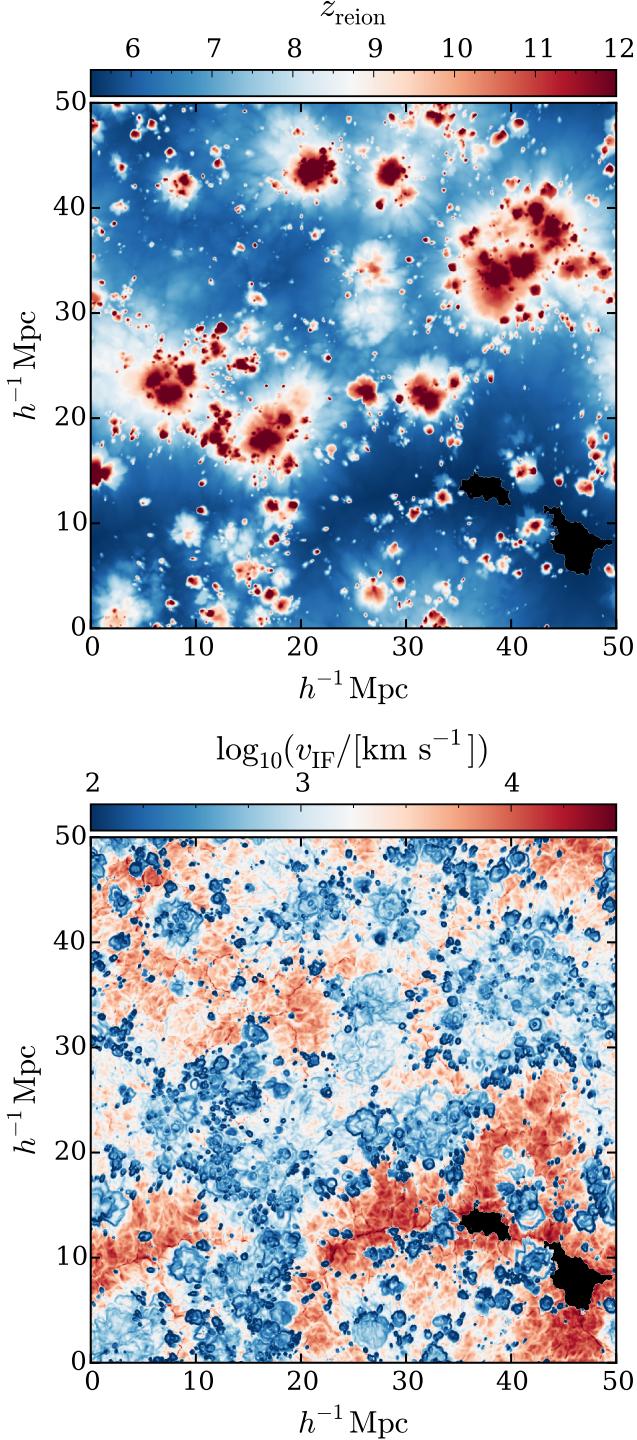


Figure 6. Top panel: a slice through the reionization redshift field in our fiducial SCORCH simulation ($\beta_{\text{esc}} = 2$). The x - and y -axes are in comoving units. The two black regions in the lower right corner correspond to last remaining patches of neutral gas in the final simulation output at $z = 5.5$. Bottom panel: corresponding slice through the field of I-front speeds obtained using the gradient method (see §3.2.2). I-fronts start out moving slowly in the over-dense regions that are reionized first. I-front speeds increase rapidly as they penetrate into under-dense voids towards the end of reionization.

The top and bottom panels of Figure 6 show a slice through the smoothed z_{re} field in our fiducial simulation, and the corresponding $|\mathbf{v}_{\text{IF}}|$ field obtained with equation (2), respectively. From these panels a strong correlation between the redshift of reionization and the local I-front speeds is evident. At the start of reionization, the H II regions expand slowly around the first sources. The speeds increase as the bubbles grow to encompass more sources, achieving their fastest speeds as they race through the under-dense regions that are reionized last. We will examine these trends quantitatively below.

Flux Method: As a cross check to the gradient method, we also estimate I-front speeds using the flux of ionizing photons at the front boundaries. We provide details for this method in Appendix C. In summary, the estimator for the I-front speed is

$$v_{\text{IF}} = \frac{cF}{F + cn_{\text{H}}(1 + \chi)}, \quad (3)$$

where $\int_{\nu_{\text{HI}}}^{\infty} F(\nu)d\nu$ is the number flux of ionizing photons at the front boundary, and the factor $1 + \chi = 1 + n_{\text{He}}/n_{\text{H}} \approx 1.08$ accounts for singly ionized Helium. We use the z_{re} fields from the simulations to identify optically thin RT cells near the I-front boundaries at a given snapshot in time. For a given boundary cell, we estimate F by counting up the number of ionizing photons within the cell. The local hydrogen number density, n_{H} , is obtained by smoothing the hydro density field to the RT resolution. The flux method overestimates v_{IF} because it assumes that all of the cell's photons propagate in a direction that is normal to the I-front. However, the worst that the local v_{IF} can be overestimated under this assumption is a factor of 2 if the radiation is impinging uniformly from all directions onto the plane of the I-front. In realistic situations the radiation is likely more directional such that the flux method provides a closer estimate to the true v_{IF} .

Lastly, we note the possibility of using equation (3), in combination with the fit of equation (1), to lay down T_{reion} values “on-the-fly” in cosmological RT simulations that would otherwise be unconvolved in T_{reion} (e.g. monochromatic simulations).

3.2.3. Results

We begin by comparing the gradient and flux methods. The top panel of Fig. 7 shows the probability distributions of v_{IF} at four snapshots in time using the gradient method on our fiducial simulation. The solid histograms in the middle panel show the flux method results at two of the redshifts for which full simulation outputs were saved. For ease of comparison, the thin/dashed histograms show the corresponding gra-

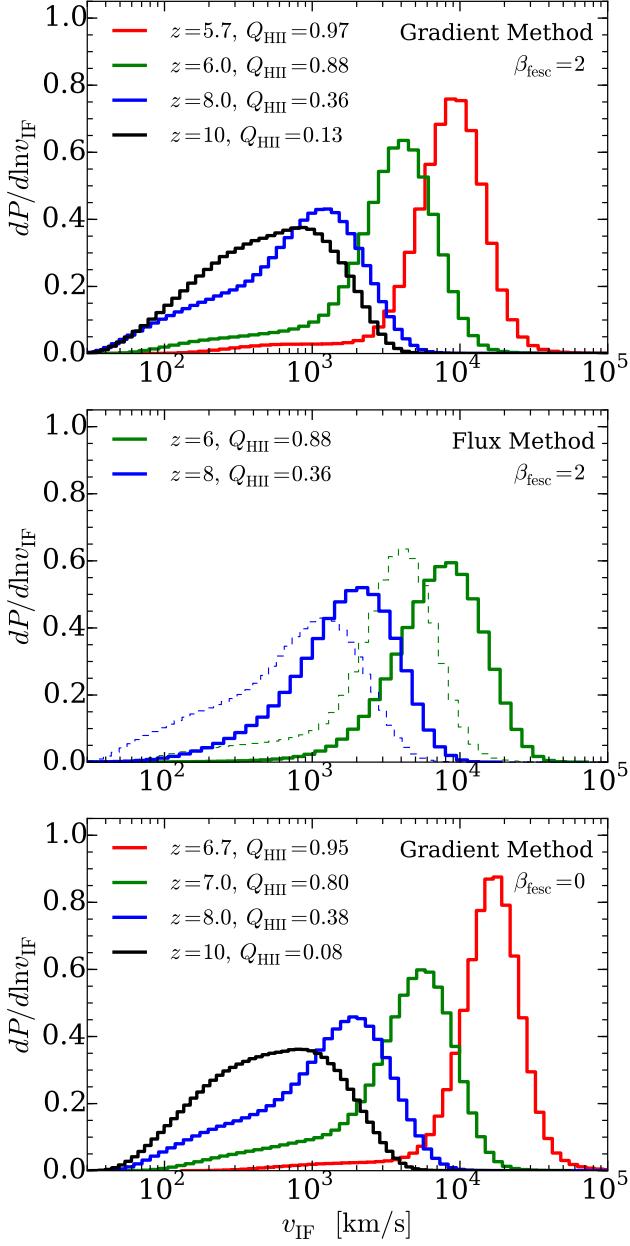


Figure 7. Distribution of I-front speeds in the SCORCH reionization simulations. From left to right, the distributions correspond to progressively later snapshots in time. The top and middle panels compare speeds in our fiducial simulation ($\beta_{\text{esc}} = 2$) obtained from the gradient and flux methods, respectively. (For ease of comparison, the gradient results are represented by thin dashed curves in the middle panel.) The bottom panel shows speeds in the $\beta_{\text{esc}} = 0$ simulation, in which the duration of reionization is shorter. I-fronts move faster in models with a shorter duration of reionization, leading to hotter post-I-front temperatures.

cient method distributions, reproduced from the top panel. We note that the results disagree by a factor of ≈ 2 , with the flux method yielding faster speeds. While this factor apparently corresponds to the maximum possible amount that the flux method can overestimate v_{IF} (as described above), we argue that this discrepancy is unlikely to result solely from the flux method limitations. It may indicate that the gradient method is also underestimating I-front speeds, perhaps due to noise in the z_{re} fields. However, the flux method is of limited utility because it can only be applied to redshifts at which we have full RT outputs. Since the gradient method allows us to obtain v_{IF} at all times using just the z_{re} field, we will adopt its slower speeds as our fiducial results, which results in somewhat lower T_{reion} .

The top and bottom panels of Fig. 7 compare the speeds in the $\beta_{\text{esc}} = 2$ and 0 simulations, where the duration of reionization is shorter in the latter. Intuitively, the shorter the duration of reionization, the faster the I-fronts must move. In both cases, the distributions are broad at early times ($Q_{\text{HII}} \sim 10\%$), spanning two orders of magnitude from ~ 50 to 2×10^3 km/s. During this phase of reionization, H II bubbles are expanding from individual (or few) sources that are typically embedded in over-dense regions of the universe. The slowest speeds in the distribution correspond to I-fronts that are retarded either by dense regions surrounding the sources, or by their episodic star formation histories. As reionization progresses, the H II regions begin to encompass more sources, such that the flux of ionizing photons at the front boundaries increases rapidly. The I-fronts break free from the over-dense regions and expand quickly through the voids. Thus we observe a strong evolution in the I-front speeds, with v_{IF} reaching $\sim 10^4$ km/s prior to overlap. These results are broadly consistent with the findings of Deparis et al. (2018), who also found a progression towards rapid speeds near overlap. In the next section, we will translate these I-front speeds to post-I-front temperatures.

4. THERMAL HISTORY OF THE IGM

In this section, we synthesize our results into a model for exploring the impact of T_{reion} on the thermal history of the IGM. Let us begin by describing a simple prescription for laying down T_{reion} values for any given z_{re} field. The first step is to apply the gradient method of §3.2 to compute $|\mathbf{v}_{\text{IF}}|$ at each location in the z_{re} field. Then, the fit of equation (1) can be used to translate these speeds to post-I-front temperatures at each location. In Figure 8 we apply this procedure to the SCORCH z_{re} fields to obtain T_{reion} distributions. Each histogram corresponds to a particular time during reionization, with

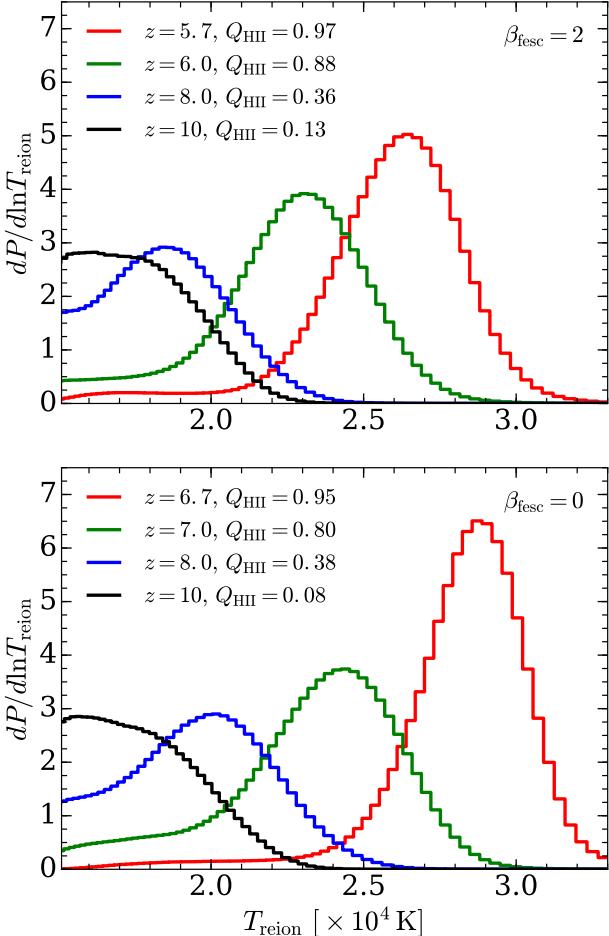


Figure 8. Models for the distribution of post-I-front temperatures during reionization. We use the fit of equation (1) to map the velocity distributions in Fig. 7 to T_{reion} values. Velocities were obtained using the gradient method and we assume a spectral index of $\alpha_{\text{IF}} = 1.5$. The post-I-front temperatures become hotter throughout reionization, with $T_{\text{reion}} \approx 25,000 - 30,000$ K near the end of this process.

redshift decreasing towards the right. The distributions are broad throughout, but the temperatures evolve significantly as reionization progresses. Post-I-front temperatures are typically around 17,000 K during the early phases of reionization ($Q_{\text{HII}} = 0.1$), but the mean values reach $T_{\text{reion}} = 26,000$ (29,000) K near the end of this process in the $\beta_{\text{sec}} = 2$ (0) models. Models with a shorter duration of reionization lead to hotter temperatures, as the I-fronts must traverse the same volume in a shorter time frame.

Next, we evolve the temperatures in time to explore what our results imply for the thermal history of the IGM. We adopt an approach similar to that of Davies et al. (2018a) and Upton Sanderbeck et al. (2016). In

this simplified model, the temperature of each gas parcel evolves according to

$$\frac{dT}{dt} = -2HT + \frac{2T}{3\Delta} \frac{d\Delta}{dt} - \frac{T}{n_{\text{tot}}} \frac{dn_{\text{tot}}}{dt} + \frac{2}{3k_B n_{\text{tot}}} \frac{dQ}{dt}, \quad (4)$$

where H is the Hubble parameter. The dQ/dt term includes H I and He I photoheating and all of the relevant cooling processes for ionized gas of primordial composition (Hui & Gnedin 1997). McQuinn & Upton Sanderbeck (2016) showed that the temperature of a gas parcel at a given density will be nearly the same for any reasonable model of its prior density evolution. For simplicity, we adopt the Zel'dovich pancake approximation for the adiabatic compression/expansion term in which $\Delta(a) = [1 - \lambda G(a)]^{-1}$, where $G(a)$ is the linear growth factor, and the constant λ is adjusted to match the simulation densities at the redshift of interest. (Here we shall consider $z = 5.5$.) For each cell in the SCORCH z_{re} fields, we set $T = T_{\text{reion}}$ at the appropriate redshift and solve the differential equation numerically to get T at a later time. There are two important caveats to this approach. First, equation (4) does not account for shock heating by collapsing structures, which will become evident when we compare our results against the full SCORCH simulation results below. Second, it is incorrect – strictly speaking – to apply this Lagrangian equation to our Eulerian gas cells. However, we will see that this simple and computationally inexpensive approach reproduces the large-scale structure of the temperature field.

Using our fiducial SCORCH run, Fig. 9 shows 2D slices of the temperature fields for three models at $z = 5.5$. We note that reionization ends at $z \approx 5.5$ in this simulation, so these slices represent snapshots of the temperature field at the end of reionization. Indeed, the black islands correspond to the last remaining patches of neutral gas. The top-left and top-right panels show models with spatially uniform $T_{\text{reion}} = 20,000$ and 30,000 K, respectively. The bottom-left corresponds to our new model for laying down T_{reion} . For comparison, the bottom right panel shows the temperature field extracted directly from the full RadHydro simulation data. First we note the higher temperatures in the filaments due to shock heating, which is not included in our simple models. It is also evident that the model with spatially uniform $T_{\text{reion}} = 20,000$ K does not capture the hottest post-I-front temperatures that are imprinted near the end of reionization. Even compared to our full T_{reion} model (bottom-left), the temperatures of recently reionized patches are somewhat hotter in the full RadHydro simulation (bottom-right). This may be a symptom of

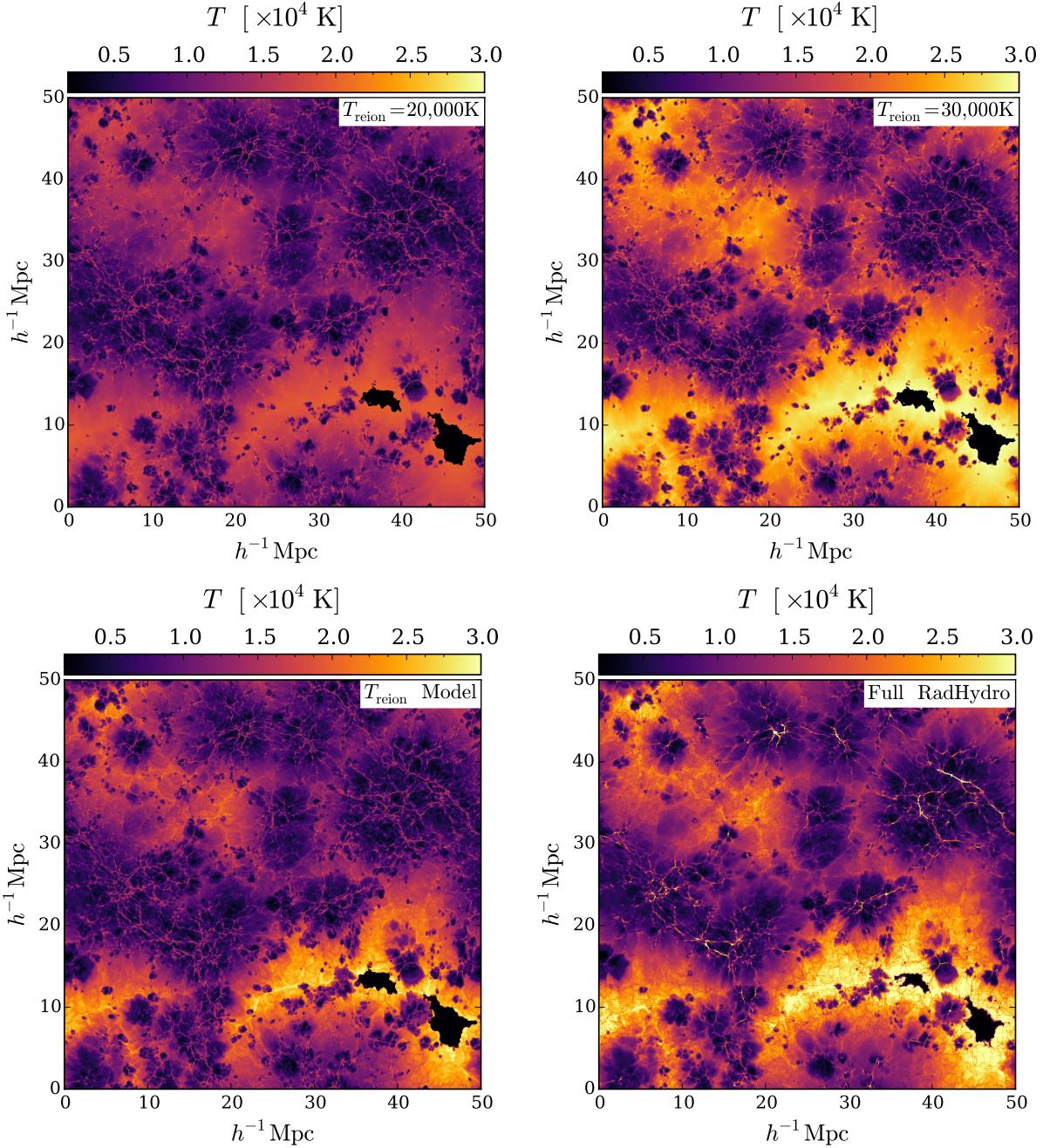


Figure 9. Slices through the temperature field at $z = 5.5$ in three models for T_{reion} (top-left, top-right, and bottom-left) compared to the temperatures in the full Radhydro simulation (bottom-right). Here we use results from our fiducial SCORCH simulation with $\beta_{\text{esc}} = 2$. The panels labeled $T_{\text{reion}} = 20,000$ and $30,000 \text{ K}$ assume a fixed T_{reion} , while the panel labeled “ T_{reion} Model” corresponds to our new model for laying down T_{reion} based on I-front velocities. The two black patches in the lower right-hand corners of the panels correspond to last remaining patches of neutral gas.

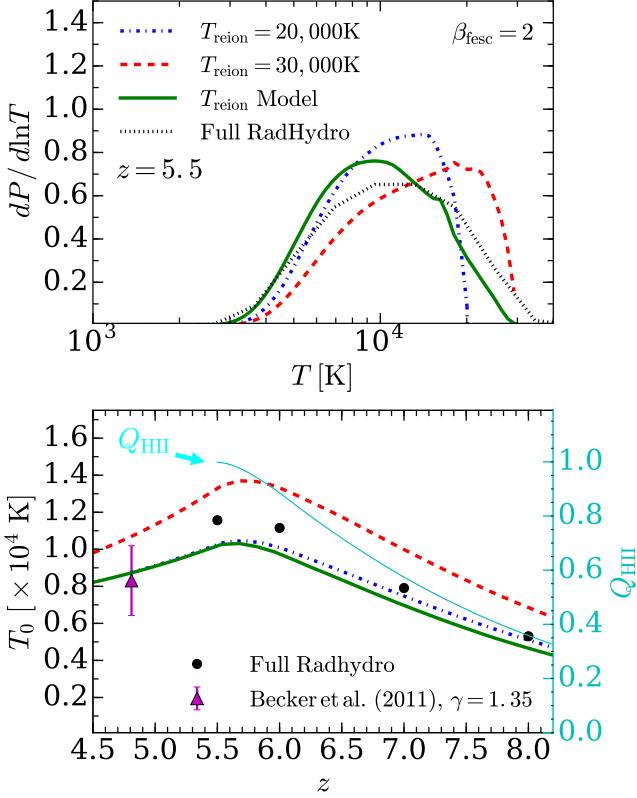


Figure 10. Effects of reionization on the thermal history of the IGM. Top panel: Distribution of temperatures (across all densities) at $z = 5.5$ in three models compared to the full Radhydro simulation results. The models correspond to those in Fig. 9. Bottom panel: Temperature at the mean gas density (T_0). The triangular data point corresponds to the measurement of Becker et al. (2011). For reference, the thin/cyan curve shows the volume filling fraction of ionized hydrogen, Q_{HII} (right axis).

the gradient method underestimating v_{IF} , or spectral filtering, which is not included in our model.

For a more quantitative look at these temperatures, the top panel of Fig. 10 shows the temperature distributions at $z = 5.5$ (across all densities). As noted above, the uniform $T_{\text{reion}} = 20,000$ K model misses the high-temperature tail of the distribution, and the full RadHydro distribution is somewhat wider than that of our model. The bottom panel examines the evolution of the temperature at the mean density of the universe in the three models. To make contact with observational results, we have included the $z \approx 4.8$ temperature measurement of Becker et al. (2011), extrapolated to the mean density using a temperature-density relation of the form $T = T_0 \Delta^{\gamma-1}$, with $\gamma = 1.35$. (We note that, at this redshift, the measured T_0 is not sensitive to the choice of γ). As expected, the uniform $T_{\text{reion}} = 30,000$ K model yields a significantly hotter mean temperature

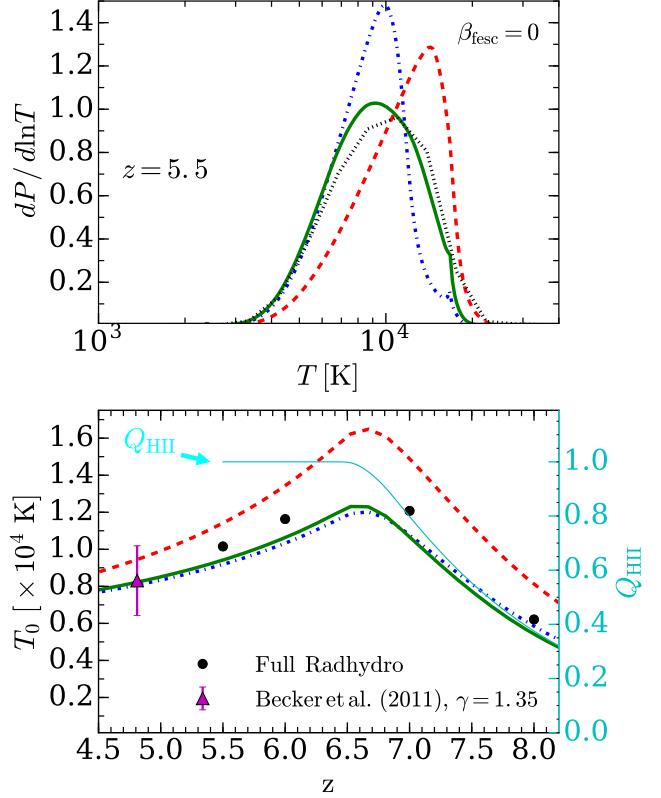


Figure 11. Same as in Fig. 10, but for the $\beta_{\text{esc}} = 0$ simulation in which the reionization epoch is shorter and ends earlier.

compared to the other models, but at $z \approx 4.8$ even this model is statistically consistent with the measurement. The top panel shows that our model for T_{reion} yields a wider distribution of post-reionization temperatures compared to the uniform $T_{\text{reion}} = 20,000$ K case. However, the bottom panel shows that the T_0 evolution for these two models is similar. This is because much of the volume in our model is, in fact, reionized to temperatures $T_{\text{reion}} \approx 20,000$ K, with the hotter values of $T_{\text{reion}} = 25,000 - 30,000$ K relegated to the fraction of the volume that is reionized late (providing the hot tail of the distribution).

Figure 11 shows the corresponding results from the $\beta_{\text{esc}} = 0$ model, which completes reionization earlier at $z \approx 6.6$. Although hotter temperatures are reached at the end of reionization in this model, the gas is somewhat colder by $z = 5.5$. The distribution of temperatures is also narrower, illustrating that the amplitude of temperature fluctuations is sensitive to the timing of overlap.

The results of this section indicate that current models of reionization yield T_{reion} as high as $25,000 - 30,000$ K near the end of this process – a consequence of the

fast I-front speeds that are achieved in these models. The range of maximum temperatures is narrower and lower, $T_{\text{reion}} = 23,000 - 25,000$ K, if the softest model considered in §3.1 (with $\alpha_{\text{IF}} \approx 2.25$) is more representative of the sources that drove the end of reionization. We note that our T_{reion} values are generally higher than those obtained in one-zone approximations of the reionization heating (see e.g. Appendix A of Puchwein et al. 2018). Such calculations do not capture the heating/cooling structure within I-fronts, which is crucial for obtaining accurate temperatures. Our maximum T_{reion} values are also higher than those found in the cosmological RT simulations of Finlator et al. (2018). Their lower temperatures – which never exceed 20,000 K – may owe to a combination of low RT spatial resolution (relative to the I-front widths) and frequency binning (K. Finlator, personal communication). It is also possible that the smaller box size used in Finlator et al. (2018) ($12h^{-1}$ Mpc) produces lower fluxes at the I-fronts, and therefore lower front velocities, particularly towards the end of reionization.

If reionization ended around $z = 6$, the hottest patches in our models could persist long enough to be detected in the $z > 5$ Ly α forest, providing a potential target for future observational studies. An important caveat here is that it is uncertain whether I-front speeds ever achieved the required speeds of $\sim 10^4$ km/s in actuality. The maximum speeds depend on the poorly understood sinks of ionizing photons at these epochs. Near the end of reionization, absorptions by self-shielding gas in the cosmic web regulate the expansion rate of H II regions (Miralda-Escudé et al. 2000; Furlanetto & Oh 2005). Current RT simulations probably have yet to achieve the spatial resolutions needed to capture this regulation effect fully, so the maximum speeds may have been slower than we find here. We emphasize that Fig. 2 provides the connection between I-front speeds and post-I-front temperatures irrespective of the reionization model. For example, if the maximum I-front speeds are revised downwards from 10^4 to 5×10^3 km/s in future simulations, Fig. 2 shows that the maximum T_{reion} would come down by $\approx 3,000$ K.

Lastly, we comment on the interpretation of the 160 comoving Mpc dark Ly α trough towards quasar ULAS J0148+0600 (Becker et al. 2015). Previous studies have invoked large ionizing background (Davies & Furlanetto 2016; Chardin et al. 2017) or temperature fluctuations (D’Aloisio et al. 2015) to explain the existence of this trough. Recently, Becker et al. (2018) conducted a narrow-band survey towards this sightline and found a significant under-density of Ly α emitters extending radially out to 30 comoving Mpc from the trough. These re-

sults indicate that the sightline intersects a cosmic void and that its Ly α opacity likely owes to a highly suppressed local ionizing background (Davies et al. 2018a). In this case, the associated void cannot be too hot without yielding detectable Ly α transmission in conflict with observed upper limits (D’Aloisio et al. 2015). There are two ways to reconcile these observations with the models presented here: either the trough was reionized much earlier than $z = 6$, or it was reionized rather slowly compared to the voids in our simulations. We note that the large-scale fluctuations that would be required to explain these observations are not captured in any reionization simulation to date, including the ones that we used here to study I-front speeds. (Nor should we expect them to be, since the fluctuations occur on scales similar to or larger than the typical box sizes of the simulations.) The currently favored model for the large-scale fluctuations requires that the mean free path be a factor of $\gtrsim 2$ shorter than extrapolations of measurements at $z \lesssim 5.2$ (Davies & Furlanetto 2016; D’Aloisio et al. 2018). If confirmed, this would imply that absorptions played an important role in regulating the reionization process. Future studies should investigate the parameter space for reionization that is consistent with this scenario.

5. CONCLUSION

We have presented a study of post-I-front temperatures during reionization. We used a suite of high-resolution RT simulations to quantify the dependence of T_{reion} on the I-front speed and the spectrum of incident radiation. We found that post-I-front temperatures are only mildly sensitive to the spectral index of the incident radiation over most of the parameter space, with T_{reion} set primarily by the local I-front speeds. The results of our parameter space study can be used to map I-front speeds to T_{reion} .

We then measured I-front speeds in cosmological RT simulations to determine what current models of reionization predict for T_{reion} . The distribution of speeds is broad during the early phases of reionization, with values ranging from 50 to 2×10^3 km/s. However, v_{IF} increases and the distribution narrows with time such that $v_{\text{IF}} \sim 10^4$ km/s near overlap. Mapping these velocities to temperatures yields $T_{\text{reion}} = 17,000 - 22,000$ K during the first half of reionization, but hotter temperatures of $T_{\text{reion}} = 25,000 - 30,000$ K are reached near overlap. A shorter duration of reionization generally implies hotter temperatures, since the I-fronts must move at faster speeds.

If reionization ended near $z = 6$, our models suggest that hot, recently reionized gas may be observ-

able in high-resolution quasar absorption spectra. In addition to being hot, these regions should exhibit a mildly inverted temperature-density relation, reflecting the slower(faster) speeds at which I-fronts move through over(under)-densities. Such regions provide a potential target for future studies pursuing signatures of reionization in high- z quasar absorption spectra. It is worth noting that a lack of evidence for hot regions would also lead to important insights on reionization. For example, their absence may indicate that reionization ended significantly earlier than $z = 6$. It is also possible that I-fronts moved at slower speeds near overlap than is predicted by contemporary models. Since the cold, pre-reionization gas clumps on scales below the resolution limits of current simulations, the poorly understood sinks of ionizing photons may not be well captured in our models. In this case, the lack of hot gas would ul-

timately provide observational insight into the role of sinks in setting the speed limit for I-fronts.

Modeling the signatures of reionization in quasar absorption spectra requires a confluence of ionizing background and temperature effects, where accurate post-I-front temperatures are a key ingredient for the latter. The results of our parameter space study can be applied to future models of the thermal history.

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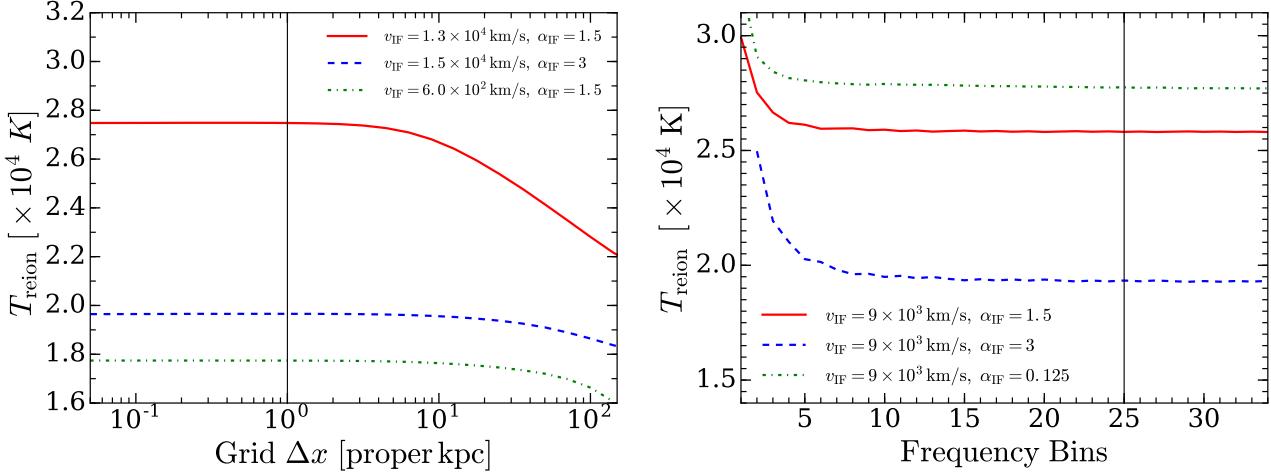


Figure 12. Numerical convergence of our 1D RT simulations. Left panel: convergence with respect to the spatial grid cell size. The curves correspond to different I-front speeds and spectral indices as denoted in the legend. The vertical line shows the cell size of 1 proper kpc chosen for all of the runs in this paper. Right panel: convergence with respect to the number of RT frequency bins. The bins are evenly spaced in log-space between 1 and 4 Ry. The vertical line corresponds to the number of frequency bins for all runs in this paper (25 bins).

APPENDIX

A. NUMERICAL CONVERGENCE AND OTHER TESTS

A.1. Convergence

Here we present numerical tests of our 1D RT simulation results. We begin with numerical convergence. The left panel of Fig. 12 demonstrates that our results are converged with respect to the spatial grid cell size, Δx . The curves correspond to T_{reion} at fixed v_{IF} and α_{IF} over a range of simulation resolutions. The vertical line shows the resolution adopted throughout the this paper, $\Delta x = 1$ proper kpc. We note at the resolution requirements for T_{reion} are most stringent for softer spectra because the I-fronts get thinner as α_{IF} increases. Thus resolving the heating/cooling processes within the I-fronts requires finer spatial resolution as α_{IF} increases. Interestingly, the plot shows that T_{reion} remains reasonably well-converged out to larger grid spacings of $\Delta x \approx 10$ proper kpc. However, we caution against interpreting this convergence test in the context of other simulation codes, as the convergence properties likely differ considerably between different numerical approaches.

In the right panel of Fig. 12, we demonstrate the convergence of our results with respect to the number of frequency bins. We divide up the spectrum into N evenly spaced frequency bins in logarithmic space. For all runs, the bins are bounded by 1 and 4 Ry, i.e. the low (high) end of the lowest (highest) frequency bin corresponds to 1 (4) Ry. The vertical line in the plot corresponds to the fiducial value of 25 frequency bins chosen for all runs in this paper.

A.2. Test of the modified RT code

As described in §2.1, we modified the code of Davies et al. (2016) to make extracting T_{reion} simpler, and to effectively define α_{IF} as the spectral index of the *incident* radiation. Here we compare our code against the original, demonstrating that they produce nearly identical T_{reion} values. Let us begin by illustrating the utility of the modified code. The solid curves in Figure 13a show the gas temperature in a simulation with the original code at three snapshots in time. The sharp boundaries correspond to the locations of the I-front as it progresses from left to right. The temperature peaks inside the I-front and the cooling behind it is driven primarily by Compton cooling and adiabatic expansion. The dashed curve corresponds to the final snapshot of a simulation with the modified code, which turns off Compton and expansion cooling, as well as all thermal evolution behind the front (but is otherwise identical to the original simulation). Note that the modified code effectively records the temperature immediately behind the I-front, i.e. the intersection of the dashed and solid curves, such that it can be simply read off from the final snapshot data. In contrast, to obtain these temperatures from the original code, we would have to locate the I-front in a given snapshot and pick off the temperature behind the front, but before the cooling processes set in. It is difficult to obtain a robust

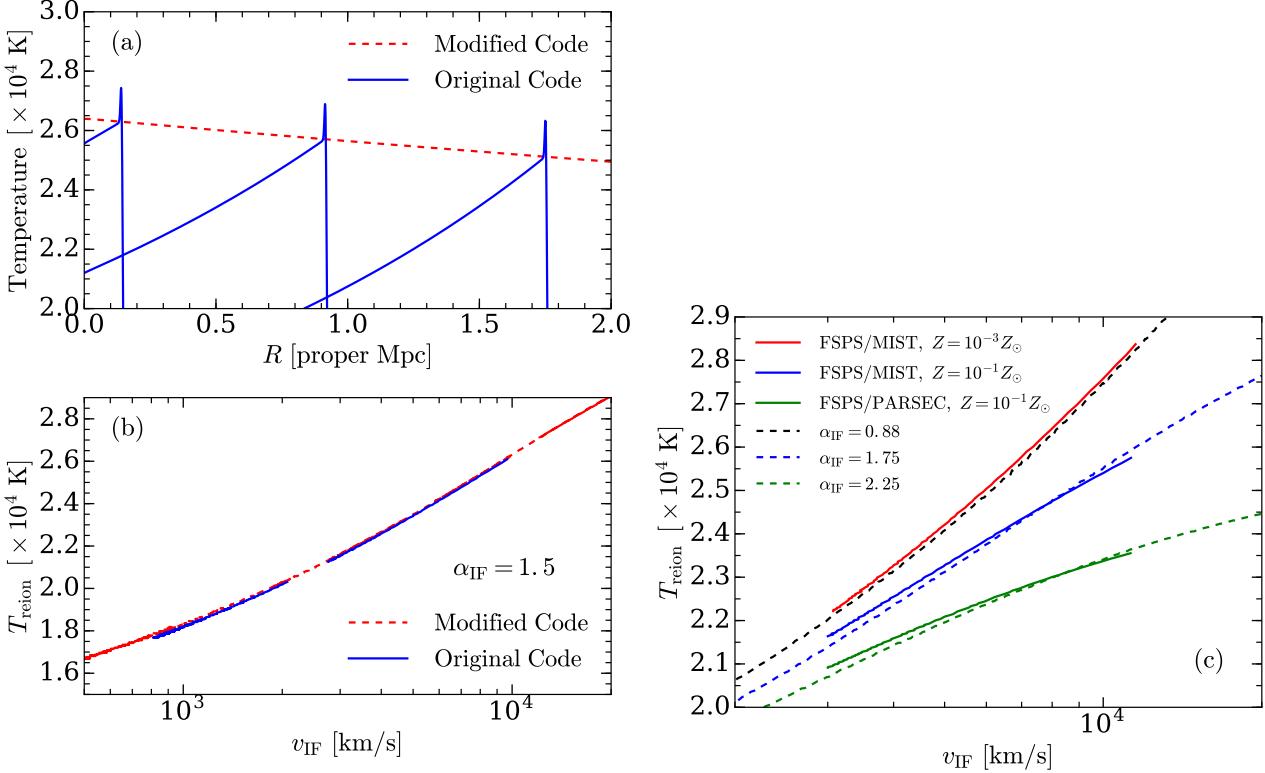


Figure 13. Tests of the 1D RT code. (a) Visual comparison of T_{reion} values obtained using the original and modified RT codes. The solid curves show the gas temperature along the line of sight obtained from the original code at three snapshots in time: from left to right, $t = 20, 100, 200$ Myrs. The dashed curve corresponds to the last snapshot of a simulation run with the modified code (but otherwise identical). The modified code turns off the thermal evolution of the gas behind the front, allowing T_{reion} to be obtained for all R at the end of the simulation. (b) Quantitative comparison of T_{reion} values. Here we compare T_{reion} vs. v_{IF} for fixed $\alpha_{\text{IF}} = 1.5$ using the original (solid) and modified (dashed) codes. (c) Post-I-front temperatures in RT runs with population synthesis model spectra. The solid curves correspond to the time-integrated FSPS spectra shown in Fig. 5. The dashed curves correspond to the simple power-law models (with sharp cutoff at 4 Ry).

prescription for doing this because the I-front widths vary significantly over the parameter space that we explore, and we must be careful to avoid the temperature structure within the I-front itself (i.e the peaks in Fig. 13a). The modified code greatly simplifies this task. In Fig. 13b, we compare T_{reion} vs. v_{IF} curves (for fixed $\alpha_{\text{IF}} = 1.5$) obtained with the original and modified codes. For the former, we record T_{reion} by extracting the temperature 10 kpc behind the peak temperature. (Visually this provides a reasonable estimate for locating the back end of the I-front in this particular case.) We note that the codes produce nearly identical results.

A.3. RT runs with stellar population synthesis models

Throughout this paper, we assume simple power-law spectra with sharp cutoffs at 4 Ry. Conveniently, this allows us to parameterize the effects of the incident spectrum in terms of the spectral index, α_{IF} . But where do the integrated FSPS spectra in Fig. 5 lie in this parameter space? To address this question, we have also performed test runs using the FSPS spectra. To make the results directly comparable to those of our power-law models, we have applied the same frequency binning to the FSPS spectra. Specifically, we re-bin the spectra into 25 logarithmically-spaced frequency bins between 1 and 4 Ry. (We note that the FSPS spectra display a steep decline at 4 Ry such that photons above this energy contribute relatively little to the ionizing background in practice.) The red and blue solid curves in Fig. 13 show T_{reion} versus v_{IF} for the MIST models with $Z = 10^{-3} Z_{\odot}$ and $Z = 10^{-1} Z_{\odot}$, respectively. The green solid curve corresponds to the PARSEC model with $Z = 10^{-1} Z_{\odot}$. The dashed curves show similar results assuming power-law spectra. For the MIST models, the post-I-front temperatures are similar to those of power-law models with $\alpha_{\text{IF}} \approx 0.88$ and 1.75 for $Z = 10^{-3} Z_{\odot}$ and $Z = 10^{-1} Z_{\odot}$, respectively. For the PARSEC model, we find $\alpha_{\text{IF}} \approx 2.25$. We note that

these are similar to the effective spectral indices that are obtained by matching the mean energy per ionization in the optically thick limit (see discussion in §3.1).

B. THERMALIZATION TIMESCALES WITHIN I-FRONT

All of our calculations assume that the timescale for photoelectrons to thermalize with the electrons, ions, and neutrals in an I-front is much shorter than the time over which the gas is within the front,

$$t_{\text{IF}} = 9.8 \times 10^5 \text{ yr} \left(\frac{R_{\text{IF}}}{10 \text{ pkpc}} \right) \left(\frac{v_{\text{IF}}}{10^4 \text{ km s}^{-1}} \right)^{-1}. \quad (\text{B1})$$

Here, $R_{\text{IF}} \sim 10$ (proper) kpc is a typical I-front width (motivated by Fig. 3), and $v_{\text{IF}} \sim 10^4 \text{ km s}^{-1}$ is a typical I-front speed in our cosmological RT simulations near the end of reionization (see §3.2). Following the discussion in the third paragraph of §2.2, $t_{\text{IF}} \propto \Delta^{-1}$ at fixed v_{IF} . The rates in the ensuing paragraph also scale as Δ^{-1} and so we drop these dependences in our expressions for equilibration times. In what follows, these times are defined as $[3/2n_X k_b T]/|dU_{XY}/dt|$ where n_X is the number density of the species of interest, X , and dU_{XY}/dt is the energy exchange rate between species X and Y , assuming X is cold and Y is at temperature T .

We find that the assumption of a fast equilibration is justified. Equilibration happens in the following sequence. First, photoelectrons stream ahead of the I-front. Their energy heats the electron bath in a short timescale, $t_{\text{photo-e,eq}} \approx 50 (E/30\text{eV})^{3/2} [x_i Z_8^3]^{-1} \text{yr}$, where we have used the maximum energy of a photoelectron of 30 eV (corresponding to the ionization of He I by a 4 Ry photon), and $Z_8 \equiv (1+z)/8$. (Little of the heat for such low energy photoelectrons goes directly into ionization or exciting atomic transitions, another assumption our calculations make. We have tested this assumption in detail.) Note that $t_{\text{photo-e,eq}}$ should be evaluated at $x_i \sim 0.5$, which corresponds to the regime within an I-front where cooling becomes important (Furlanetto & Stoever 2010). The thermalized electrons then give their energy to the ions over again a relatively short timescale of $t_{\text{e-p,eq}} \approx 3000 T_4^{3/2} [x_i Z_8^3]^{-1} \text{yr}$, where $T_4 \equiv T/[10^4 \text{ K}]$. Lastly, the neutrals are heated primarily by collisions with protons. At the relevant temperatures, the collisional processes are dominated by resonant exchange of electrons (allowing e.g. hot ions to become hot neutrals as the kinetic energy is maintained), which we find is an order of magnitude more important than non-resonant collisions. The equilibration timescale of the neutrals is $t_{nI} \approx 40,000 T_4^{-1/2} [x_i Z_8^3]^{-1} \text{yr}$ (Rapp & Francis 1962; Banks 1966), which is safely smaller than t_{IF} for all but the most relativistic speeds.

C. ESTIMATING I-FRONT SPEEDS FROM PHOTON FLUXES

In this section, we describe an alternative method for estimating I-front speeds in cosmological RT simulations. Consider a plane-parallel I-front moving at speed v_{IF} with respect to the frame of the gas. The front is driven by impinging radiation with spectrum $S(\nu)$ and photon number flux, $F = \int_{\nu_{\text{HI}}}^{\infty} d\nu S(\nu)$, where ν_{HI} corresponds to the ionization threshold of hydrogen. An observer in the rest frame of the I-front will observe the influx of neutral atoms on one side of the front perfectly balanced by the flux of ionizing photons on the other side, $\mathcal{F} = (1-v_{\text{IF}}/c) \int_{\nu_{\text{HI}}}^{\infty} d\nu S(\nu)$. Thus, the front velocity obeys,

$$\mathcal{F} = n_{\text{H}}(1+\chi)v_{\text{IF}}, \quad (\text{C2})$$

where n_{H} is the proper hydrogen number density, and the factor, $1+\chi$, accounts for the ionization of helium. Here we assume that helium is singly ionized, in accordance with standard models of the reionization process, in which case $1+\chi = 1+n_{\text{He}}/n_{\text{H}} \approx 1.08$. From equation (C2), our estimator for the magnitude of the I-front velocity is

$$v_{\text{IF}} = \frac{cF}{F + cn_{\text{H}}(1+\chi)}. \quad (\text{C3})$$

In §3.2, we use equation (C3) to calculate the distribution of v_{IF} at a given epoch. For a given z , we first use the z_{re} field to locate RT cells at the boundaries of the I-fronts, i.e. cells that are reionized between z and $z + \delta z$. In what follows, we use $\delta z = 0.02$, but we have tested that our results are insensitive to the exact choice. Since equation (C3) applies only in the limit of a sharp I-front boundary, we further select from the recently reionized cells those that have neutral hydrogen fractions $x_{\text{HI}} < 0.01$ to avoid optically thick cells. (Again, we have verified that our results are not sensitive to variations in the exact value of this threshold.) We then compute the number flux F in the selected cells using

$$F = \frac{\Delta l_{\text{rt}}}{\Delta t_{\text{rt}}} \sum_{i=1}^{N_{\text{freq}}} n_{\gamma,i}, \quad (\text{C4})$$

where $n_{\gamma,i}$ is the photon number density in the i th frequency bin, Δl_{rt} is the proper RT cell length, and Δt_{rt} is the RT time step. To obtain n_{H} , we smooth the n_{H} field (which is stored at the hydro resolution) to the RT grid resolution by convolving with the coordinate-space top-hat function. We have tested the accuracy of the above procedure against the results of a 1-dimensional version of the RadHydro code, in which the velocities of I-fronts can be directly measured. We find excellent agreement for all cases tested, including runs in which we vary the speed of light from $c_{\text{sim}}/c = 0.1$ to 1.