Radiative transfer of ionizing radiation through gas and dust: stellar source case

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ABSTRACT

We present a new dust extension to the Monte Carlo radiative transfer code CRASH, which enables it to simulate the propagation of ionizing radiation through mixtures of gas and dust. The new code is applied to study the impact of dust absorption on idealized galactic H II regions and on small scale reionization. We find that H II regions are reduced in size by the presence of dust, while their inner temperature and ionization structure remain largely unaffected. In the small scale reionization simulation, dust hardens ionization fronts and delays the overlap of ionized bubbles. This effect is found to depend only weakly on the assumed abundance of dust in underdense regions.

Key words: radiative transfer – ISM: dust, extinction – cosmology: dark ages, reionization, first stars

1 INTRODUCTION

The existence of cosmological dust in the diffuse Galactic interstellar medium (ISM) was first inferred from the extinction of starlight (Trumpler 1930). Since that time, much observational evidence of dust has been found, for example in star-forming regions (e.g. Churchwell et al. 2009) or our Solar System (e.g. Srama et al. 2011), and it has become increasingly apparent that, at least in collapsed structures, dust is ubiquitous in the Local Universe.

One of the best-studied properties of dust is its wavelength dependent extinction (e.g. Fitzpatrick 1999). Although the exact dependence varies from environment to environment, a very general finding is that dust preferentially absorbs visible and ultra-violet (UV) light (e.g. Draine 2011a). Though observationally less well constrained, models predict a large dust cross section also in the ionizing UV (13.6–200 eV; see § 3.2).

The former point has important consequences for the observation of recent star formation, traced by massive and short-lived stars, which emit most of their energy in the UV (e.g. Kennicutt & Evans 2012). These stars are observed to form in groups (OB associations) in dense, dusty molecular clouds (e.g. Garay & Lizano 1999; de Zeeuw et al. 1999), so that a large fraction of their radiation is often absorbed by dust, which re-emits in the infra-red (IR), impeding direct observation of the star formation process and strongly changing galaxy colours (e.g. Mancini et al. 2016; Lewis et al. 2017).

The latter point has interesting implications for the formation of H II regions by ionizing UV radiation, one of the feedback channels of massive stars on the ISM. Despite a long series of studies investigating their spectral line diagnostics: structure, evolution and physical status of the ionized gas in these regions still remain subjects of intense theoretical and observational activity (see e.g. O’Dell 2001; Whitney et al. 2004; Purcell et al. 2009; Winston et al. 2011; O’Dell et al. 2017). Galaxies of the Local Group offer a wide range of H II regions accessible at a level of detail comparable to Galactic observations (Kennicutt 1984; Massey & Hunter 1998), but located in differing ISM environments, e.g. with quiescent star formation as observed in M31 (Azimlu et al. 2011) or M33 (Relaño et al. 2016). Beyond the Local Group a large statistical sample of star forming galaxies can also be studied at the price of resolving less details, but with the advantage of investigating a wider variety of active star forming environments (Gilbert & Graham 2007).

The connection between the size of H II regions and their electron number density (the so called size-density relation) in observational samples has been investigated as tracer of the physical status and structure of their ISM (see Hunt & Hirashita 2009; Draine 2011b and references therein). Dust certainly plays a role in shaping this relation and has been recognized as crucial to its deviation from pure Strömgren sphere (Strömgren 1939) expectations (e.g. Inoue et al. 2001; Arthur et al. 2004).
Understanding dusty H\textsc{ii} regions is therefore important in the context of star formation; it is, however, also closely linked to understanding the reionization of the Universe. The importance of the role galaxies played in this process depends on what fraction $f_{\text{UV}}$ of the ionizing UV radiation they produce escapes to the intergalactic medium (IGM) (Madau et al. 1999; Meiksin 2009; Wilding et al. 2013). Dust presumably influenced $f_{\text{UV}}$, since several galaxies observed in the epoch of reionization (EOR) appear to be dusty (e.g. Watson et al. 2015; Willott et al. 2015; Laporte et al. 2017), indicating that grain populations were present already during the EOR.

3D radiative transfer (RT) simulations are the most powerful tool available to theorists to investigate this topic. Very capable codes have been written and, in some cases, published for dust RT (e.g. Steinacker et al. 2013; Gordon et al. 2017), gas RT (which recently is often coupled to hydrodynamics, e.g. Bisbas et al. 2015a) and gas RT on cosmological scales (e.g. Iliev et al. 2006, 2009)\footnote{Note that, since the literature for each of these areas is vast, we only cite a few reviews or comparison papers.}. However, while the spectral synthesis code CLOUDY (Ferland et al. 2017), or other photon dominated region codes (for a comparison of several of them see Röllig et al. 2007) have included dust effects for many years, dust and gas are generally not treated together in 3D RT codes. We are aware of the following exceptions: MOCASSIN (Ercolano et al. 2005), the code used in Wood et al. (2010), ART\textsuperscript{2} (Yajima et al. 2012), SEDNA (Bisbas et al. 2015a, § 3.9) and TORUS-3DPDR (Bisbas et al. 2015b), all of which are gas RT codes that feature dust physics and chemistry models of varying complexity. Recently, gas and dust RT have also been coupled in the modelling of protoplanetary discs. Taking advantage of the symmetry of the problem, these codes are, however, generally 2D (e.g Woitke et al. 2009; Bruderer et al. 2014).

As explained above, dust is often present where ionizing photons are produced, and it will compete with the gas for their absorption (see also § 3.2). The emission of photoelectrons from dust can significantly contribute to gas heating (Draine 2011a) and introduces a direct coupling of gas and dust via a shared free electron pool. We therefore believe it is important to be able to treat RT through gas and dust simultaneously.

Here we perform a first step towards this goal by applying a newly extended RT code to model the impact of the ionizing radiation emitted by a single young O-type star in the Local Universe on a dust-polluted medium\footnote{Analytic solutions for this problem have been published in the literature (e.g. Petrov et al. 1972) and we compare our code against them in Appendix A.}. In this context we also evaluate the contribution of PAHs to dust absorption at ionizing photon energies. We furthermore investigate the effect of dust in the early Universe on small scale reionization by artificially polluting a small cosmic web. This is done in preparation of future applications we envision for our code, one of which is studying the impact of dust production on the evolution and detectability of high redshift objects and their surroundings. For the time being, we consider only the absorption of ionizing photons by dust.

This paper is organized as follows: in § 2 we describe CRASH, the 3D RT code used to simulate ionization of hydrogen and helium gas, which we extended by a dust module. In § 3 we describe the dust model we use and provide details on the implementation. § 5 contains our results and in § 6 we present our conclusions.

2 CRASH

CRASH (Cosmological Radiative transfer Scheme for Hydrodynamics) is a 3D code developed specifically to study time dependent radiative transfer (RT) problems in cosmology. The Monte Carlo (MC) algorithm it adopts enables accurate modelling of radiation-matter interactions (generally for photon energies $\nu \geq 13.6$ eV) and allows to add new interaction processes relatively easily. In its first version (Ciardi et al. 2001), the code follows hydrogen ionization by point sources, taking into account radiation emitted during recombinations. The physics of helium, a treatment of the gas temperature and the possibility to include diffuse background radiation were introduced later (Maselli et al. 2003), as well as an improved multi-frequency scheme (Maselli et al. 2009). The latter version is referred to as CRASH 2. In Graziani et al. (2013) CRASH 3 was introduced, featuring the physics of atomic metals, several improvements necessary to account for different source populations in reionization simulations (Kakiichi et al. 2017; Eide et al. 2018), optional coupling with hybrid pipelines of galaxy formation (Graziani et al. 2015; Graziani et al. 2017) and the capability to propagate photons through multi-scale AMR grids (Harrahan et al. 2017). The newest version, CRASH 4 (Graziani et al. 2018), self-consistently treats ionization by high-energy photons (up to $\nu = 10$ keV) as well as secondary ionization by collisions with high-energy photo-electrons. The name CRASH will hereafter be used to refer to this version. Most of the features mentioned in this paragraph can easily be turned on or off for a particular simulation, depending on the problem at hand.

We will now briefly describe CRASH by showing its workflow on the basis of an example simulation that does not include metals or dust and does not feature background radiation. The changes made to this workflow to account for dust are discussed afterwards. The interested reader is referred to the literature cited above for more details.

The starting point of a CRASH simulation is a set of initial conditions (ICs) provided on a three-dimensional Cartesian grid of $N_x^3$ cells and a given linear size $L_h$. The basic configuration requires:

1. number density of the gas $n_g \left[ \text{cm}^{-3} \right]$, as well as hydrogen and helium number fractions;
2. gas temperature $T$ [K] and ionization fractions $x_{\text{HI}}$, $x_{\text{He}}$, $x_{\text{He}}$ at the initial time $t_0$;
3. coordinates, emission rates of ionizing photons ($N_\lambda$) and spectral energy distributions (SEDs) of all point sources $j$;
4. the simulation duration $t_s$ and its starting redshift.

ICs can either be manually created to perform tests, or they can be obtained from N-body or hydrodynamics simulation snapshots providing realistic configurations at fixed times. RT simulations are then performed in post-processing by propagating photons through a single snapshot, or, e.g. in
the case of reionization simulations, by running CRASH successively on a set of snapshots, propagating the generated outputs from one to the next (e.g. Ciardi et al. 2003, 2012; Graziani et al. 2015; Eide et al. 2018). During a single RT run gas dynamics are not followed, but the density evolution of the gas due to cosmological expansion as well as the cosmological redshift of the propagated photons can be taken into account.

Once a set of ICs is loaded, CRASH starts looping over the point sources, emitting and propagating a photon packet from every source, until the specified number of packets per source $N_p$ is reached. The photon count of each packet is given by the source emissivity and the simulation time:

$$N_j = \frac{N_p j_l}{N_p}.$$  

(1)

These photons are distributed over user specified frequency bins in accordance with the SED of the source $j$. The emission direction is determined by randomly sampling the corresponding angular probability distribution function. Each packet is then moved along the ray specified by its direction and the source position. For every cell it crosses, the number of photons $N_v$ in a frequency bin around $v$ is reduced by

$$\Delta N_v = N_v (1 - e^{-\tau_v}),$$  

(2)

where $\tau_v = \sum_i \tau_{i,v}$ with $i \in \{\text{H I, He I, He II}\}$ is the total optical depth of the cell at frequency $v$. The partial optical depths are given by

$$\tau_{i,v} = n_i \sigma_{i,l} ,$$  

(3)

where $n_i$ and $\sigma_{i,l}(v)$ are, respectively, number density and absorption cross section of species $i$, and $l$ is the geometrical path casted by the ray through the cell. The absorbed photons are distributed among the different species in the cell according to

$$\Delta N_{i,v} = \frac{\tau_{i,v}}{\tau_v} \Delta N_v.$$  

(4)

This is used to compute ionization fractions and gas temperature (see original papers for more details).

Finally, the photon packet is moved to the next cell crossed by its ray and the process is repeated until the packet is eventually depleted or it leaves the computational domain (although periodic boundary conditions can be enabled). Photon packets created by recombination processes are emitted from the corresponding cells when the emission criteria specified in Maselli et al. (2003) are met and are treated in the same way as the photon packets emitted by a point source.

Finally note that, while Pierleoni et al. (2009) introduced an implementation of the code treating the propagation of Ly$\alpha$ photons self consistently with the ionizing continuum (by including both absorption and scattering), the code version adopted here does not feature any line scattering physics, so that it is not applicable to high density plasmas. Also note that in this work the atomic metal functionality of CRASH is not coupled with the dust module (see § 3.2).

3 DUST MODELS

Studying radiative transfer through dust and assessing its interplay with ionized gas requires detailed knowledge of several dust properties, for example optical coefficients, charging yields and sublimation temperatures. Much remains unknown about cosmic dust in general, and there is, as of yet, no consensus in the community on the composition and nature of dust even in the galactic ISM. Consequently, many different models exist (e.g. Li & Greenberg 1997; Zubko et al. 2004; Jones et al. 2013). For this reason a numerical implementation of dust in a radiative transfer code should be model-independent (see § 4).

Moreover, there is no a priori reason to assume dust at high redshift to be like the dust we observe in the local universe; in fact, evidence to the contrary has been presented (e.g. Kulkarni et al. 2016). Likewise, one should expect grain properties to vary depending on their environment (cf. Fig. 1). In the context of this work, we will only briefly investigate the processing of dust in H I regions.

This section is organized as follows. We first present the dust properties we require in § 3.1 and then introduce the Silicate-Graphite-PAH model in § 3.2, § 3.3, finally, discusses the contribution of PAHs to the dust optical depth.

3.1 Optical properties

Photon absorption and scattering by a dust grain are characterised by its frequency-dependent absorption and scattering cross sections, $\sigma_{a}(v)$ and $\sigma_{s}(v)$ respectively. $\sigma_{e} = \sigma_{a} + \sigma_{s}$ is referred to as the extinction cross section, and the relative importance of scattering against extinction is quantified by the albedo $\tilde{\omega} = \sigma_{a}/\sigma_{e}$. The scattering asymmetry parameter $(\cos \theta )$, where $\theta$ is the scattering angle and the brackets indicate averaging over scattering events, complements the information about the capability of dust grains to deviate incoming light. We customarily refer to the above-mentioned quantities as the optical properties of dust (see Henning & Mutschke 2010 for a recent review or Bohren & Huffman 1983 for an extensive treatment). They generally depend on a series of grain properties (e.g. chemical composition, solid-state structure, morphology) and environment-dependent conditions (e.g. dust temperature, charge state) and can be determined both theoretically (e.g. Draine 2003b,c) and experimentally (e.g. Henning & Mutschke 2010 or see the Amsterdam-Granada light scattering database).

Typically, the optical properties of cosmic dust can observationally only be constrained at photon energies $h\nu < 13.6\text{eV}$ (e.g. Cardelli et al. 1989), where the gas component of the ISM does not dominate absorption, and at energies $\gtrsim 10^2\text{eV}$, by means of X-ray scattering haloes (e.g. Smith & Dwek 1998; Draine & Tan 2003). In the ionizing-UV band 13.6-200eV, which is of central importance to the ionization of the hydrogen and helium gas components, one generally has to fully rely on predictions from theoretical models supported, when available, by laboratory experiments.

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3 This has been changed since Maselli et al. (2003); see also Friedrich et al. (2012, Appendix D).

4 http://www.iaa.es/scattering/
3.2 The Silicate-Graphite-PAH model

We adopt optical properties provided by the so-called Silicate-Graphite-PAH model (Weingartner & Draine 2001b and Li & Draine 2001; hereafter WD01 and LD01 respectively). In this subsection we summarize the main assumptions of the model and present some of its results, as they are necessary to understand the implementation in CRASH. We refer the interested reader to the original papers for more details.

WD01 and LD01 assume a dust composition consisting of two chemically distinct grain populations: one based on silicate and one based on carbon. For each population, they assume a grain size distribution described by a modified power-law with a smooth cut-off at large sizes (a ~ 1–10 μm) and a variable slope towards the small-size cut-off at 3.5 Å (see eqs. 4–6 in WD01). Silicate grains and large carbon grains (with an effective grain radius a ≥ 100 Å; see Weingartner & Draine 2001a, § 2.1) are assumed to be spherical and composed of olivine and graphite respectively; their optical properties are computed in the framework of Mie theory (e.g. Bohren & Huffman 1983). For the carbonaceous population two log-normal distributions peaking at 3.5 Å and 30 Å are added to provide additional small grains. Small carbon grains (a ≤ 20 Å) are given the optical properties of polycyclic aromatic hydrocarbons (PAHs), and transitional properties are used for intermediate size carbon grains (see also Eq. (B1)). WD01 and LD01 tune their size distributions in order for their dust model to reproduce the observed dust extinction and infrared emission of the diffuse Milky Way ISM. The Fitzpatrick (1999) R_V-parametrization of the extinction curve with R_V = 3.1 is chosen to represent the observed extinction, where R_V = A_V/E(B – V) is the ratio of visual extinction to reddening. The model can also reproduce extinction along many other lines of sight through the ISM of the Milky Way and also of the Magellanic Clouds, where typical extinction differs from that of our galaxy (see § 3.2 of WD01).

A later version of the model (Draine 2003a,b,c) provides corrected dust abundances as well as updated material constants. The optical properties of the dust mixture are computed in a wide energy range (~ 10^{-4}–10^4 eV), using anomalous diffraction theory (van de Hulst 1957) instead of Mie theory at X-ray energies. These new data\(^5\) are plotted as functions of photon energy in Fig. 1 for R_V = 3.1, 4.0 and 5.5. More specifically, we adopt the WD01 case A size distributions with carbon abundance per H atom in the log-normal populations h_C = 60 ppm and total carbon dust abundance corrected by a factor 0.93 for R_V = 3.1, with h_C = 40 ppm corrected by 1.18 for R_V = 4.0 and with h_C = 30 ppm corrected by 1.42 for R_V = 5.5 (see WD01 and Draine 2003a). While the three lines differ, their qualitative behaviour is very similar, and thus we will restrict ourselves to discussing the R_V = 3.1 case. We also restrict the discussion to H-ionizing energies (hν ≥ 13.6 eV) as CRASH performs RT only in this photon energy range. Note, additionally, that more recent cross sections and material constants, taking into account new observations and laboratory data, have been published for the carbonaceous model-grains (Draine & Li 2007; Draine 2016). These latest updates are not taken into account here, since the older optical data plotted in Fig. 1 are readily available and easily sufficient for the purposes of this work.

The albedo (top panel) starts out at a value of ~ 0.2 around 13.6 eV and remains below ~ 0.5 in the entire UV regime (13.6 eV < hν ≤ 200 eV), i.e. dust absorption dominates scattering at these energies. Entering the soft X-ray domain (0.2 keV < hν < 3 keV), it rises approximately linearly with log(hν) to ~ 0.6 at 300 eV. From this point onwards up to 3 keV it remains roughly constant on average, but

\(^5\) The properties used are guided by laboratory measurements and therefore the actual geometry of the PAHs is irrelevant for this purpose. When modelling aspects where this is not true, small PAHs are usually assumed to be planar while larger ones are assumed to be spherical (e.g. Hoang et al. 2010).

\(^6\) New and old data are available online at www.astro.princeton.edu/~draine/dust/dustmix.html.
so that at these energies more than 50% of the photon-dust interactions are scattering events. The scattering asymmetry parameter (second panel) rises quickly from ≈ 0.7 at 13.6 eV to unity at 100 eV, i.e. in our energy regime the dust grains are mostly to purely forward scattering.

As CRASH currently neglects scattering in its ray tracing algorithm\(^7\), we investigate the impact of this approxima-
tion using \((1 - \cos \theta) \bar{\omega}\) (third panel). This parameter measures how strongly photons are deviated from their initial direction of propagation upon interacting with a grain. If it is zero, no deviation takes place and scattering can safely be neglected. In the range 13.6 eV–3 keV, it remains below 0.1, indicating that neglecting scattering is an acceptable approximation in our ray-tracing scheme, at least with the present dust model and in applications to diffuse gas, as those of our interest. This scheme is, on the other hand, not appropriate to model protoplanetary discs, for instance, and using a different dust model might invalidate our argument. We plan to address scattering in a future release after implementing other dust processes that directly impact grain charging and gas ionization.

The bottom panel of Fig. 1, finally, shows the absorption cross section per dust mass. It peaks at ~ 17 eV (i.e. between the H\(^i\) and He\(^i\) ionization potentials) and progressively decreases with increasing energy, showing some structure owed to the inner shells of grain constituents.

Since the main goal of our implementation is to investigate the RT through dust and gas (H, He), it is important to compare the relevant cross sections at fixed photon energy. Fig. 2 shows the dust absorption cross section (dash-dotted orange) together with the ionization cross sections of neutral hydrogen (solid black) and neutral helium (dashed red) (Verner et al. 1996); these are the primary species competing with dust grains in absorbing ionizing photons. The cross sections are normalized per H nucleus. We assume protosolar gas composition (Draine 2011a, Table 1.4; see also Asplund et al. 2009) and a gas-to-dust mass ratio (GDR) of 124, as suggested by WD01 and LD01 for the diffuse ISM of our galaxy. With the above assumptions, it is evident that in a neutral gas-dust mixture, dust will only be relevant to absorption at energies of several hundred eV, but note that the GDR can vary strongly from ~ 10 to ~ 10\(^6\) (e.g. Vuong et al. 2003; Draine et al. 2007; Sandstrom et al. 2013; Rémy-Ruyer et al. 2014; Lisseau et al. 2015; Owen & Barlow 2015; Mancini et al. 2016), depending on the galactic environment. Unlike gas (which becomes ionized and thus transparent), however, the opacity of dust in photo-ionized regions does not change significantly in time unless the UV field is strong enough to destroy the grains\(^8\). Therefore dust can provide time-persistent opacity over a wide photon energy range and might be an important contributor to absorption also at lower energies. For example, a typical stellar radiation field can easily ionize both H\(^i\) and He\(^i\) so that the dust grains will, after a certain point in time, compete only with singly ionized helium (dotted blue) while continuously absorbing energy from the UV field in 13.6–54.4 eV. In reality, however, the situation is much more complex because (i) the presence of atomic metals in the gas mixture (for a discussion including abundance constraints on dust models see Draine 2003a, 2011a) alters the total optical depth and (ii) the ionization fractions and recombination rates of each species are complex functions of local conditions. It is thus not possible to make a general quantitative statement on the importance of dust absorption in ionized gas without detailed numerical modeling. We defer a more detailed discussion and the inclusion of gas phase metals to future investigations.

Our choice of the Silicate-Graphite-PAH model for the purposes of this work is owed to the fact that it is widely used, easily accessible and comparatively simple. On the other hand, this model is primarily designed to explain the various spectral features of dust extinction curves and dust IR emission on an observation by observation basis, i.e. it offers no straightforward formalism to model the evolution of a given dust population. For example, the PAH contribution to the total absorption cross section can not easily be isolated. As PAHs are susceptible to photo-dissociation, it is important to quantify the error introduced by assuming their continuous presence during the RT process. This point is addressed in the following section.

\(^7\) We repeat here that the implementation of radiation scattering in a code accounting for gas ionization and temperature as well as dust as function of time, would severely increase the computational requirements of a single run or even impede reionization simulations. Sophisticated implementations of radiation scattering on dust grains exist (e.g. Camps & Baes 2015; Gordon et al. 2017) but they are generally limited to time independent algorithms and do not account for the gas component.

\(^8\) It should be noted that this is not generally true. In molecular regions (which we do not study here), e.g., photo-detachment from negatively charged grains can appreciably change the grain cross section (e.g. Weingartner & Draine 2001a). Also note that grain destruction is not yet implemented in CRASH (see § 4) and that different grain types (both size and composition) are expected to behave very differently when exposed to radiation.
3.3 Contribution of PAHs to the dust optical depth

Dust mixtures are known to be sensitive to both UV radiation and gas phase transitions from neutral to ionized. The PAH component, in particular, is susceptible to restructuring and destruction via photo-dissociation (e.g. Voit 1992; Jochims et al. 1994; Le Page et al. 2001) and collisions with free electrons and ions present in a hot, ionized gas (e.g. Micelotta et al. 2010a,b; Böochio et al. 2012). The efficiency of the above processes, however, as well as the change in PAH composition induced by them, are not fully understood and are subject of thorough investigations (e.g. Zhen et al. 2016). Observations, nevertheless, suggest PAHs to be systematically depleted in galaxies hosting an active galactic nucleus (AGN) (Roche et al. 1991; Smith et al. 2007; Jensen et al. 2017) or in H II regions (e.g. Kassis et al. 2006; Whelan et al. 2013; Stephens et al. 2014; Salgado et al. 2016; Chastenet et al., in prep.), so that they seem to provide conditions conducive to PAH destruction (but see Compiègne et al. 2007).

While many processes of PAH evolution have been implemented for circumstellar disks (Visser et al. 2007; Siebenmorgen & Krügel 2010) or to model specific features of galactic H II regions (Giard et al. 1994), a consistent time dependent RT approach including dust mixtures and gas is still missing. It is, in fact, not clear how current models for dust mixtures (see section above) should be modified to derive cross sections excluding the photo-dissociated PAH component.

In this work we perform a first step in this direction by recomputing the cross section of a dust mixture without the PAH component in the framework of the Silicate-Graphite-PAH model. The result will be used in § 5.1.1 to assess the impact of the PAHs on the size of ideal dusty H II regions and in § 5.2 with a more complex dust distribution and source configuration.

For an immediate comparison with the discussion of the previous section, here we discuss the resulting absorption cross sections, while the details of the modelling are deferred to Appendix B.

Fig. 3 shows the dust absorption cross sections (per mass of full dust mixture) as a function of photon energy. Before introducing any changes in the dust composition, we note that the original Silicate-Graphite-PAH model with $R_v = 3.1$ (solid black line) and our own result when PAHs are included (dashed red line) are in good agreement, with a maximum difference of 9% at 21.5 eV.

A significant reduction of the cross section by a factor of two (orange line, cut model) or three (blue and green lines for split and $b_C = 0.0$ ppm, respectively) relative to the original data is found at its peak ($\sim 17$ eV) and it remains considerable ($\sim 20\%$) in the energy range up to 30 eV. The differences progressively decrease to 5% at $\sim 60$ eV, and remain at or below this value at higher frequencies because all size distributions converge to the original model, i.e. the PAH component does not contribute significantly anymore to the mixture cross section.

In summary, the PAH component provides an important contribution in absorption in the photon energy range 13.6–60 eV, while its presence is negligible in the remaining part of the spectrum. In § 3 we investigate the impact of this on gas ionization and temperature, using the $b_C = 0.0$ ppm approach to obtain an upper limit on the impact.

4 NUMERICAL IMPLEMENTATION OF DUST IN CRASH

Here we describe the modifications which enable CRASH to account for dust absorption in RT simulations. We start discussing how we abstracted this problem to achieve an implementation that is extendable and independent of any specific dust model.

The most general way to obtain the necessary data from a dust model is by interpolation of pre-computed tables, which is therefore our method of choice. Any chosen dust model might provide properties for a predefined mix of dust species (as the Milky Way model introduced earlier), or it might provide properties for individual dust species; it is therefore clear that a general dust RT code should support the concept of dust species. Furthermore, in realistic applications dust will not be distributed homogeneously in space, and its properties (composition, ionization, grain size, tem-
perature, etc.) may also be functions of location and time. An RT code accounting for dust, therefore, needs to be able to track not only the dust abundance but also its properties, possibly per species, at each point of the discretised domain during the entire RT process. This has the additional advantage that radiation effects on dust grains (such as heating, ionization, metamorphism and destruction) can be accounted for in detail, and their coupling to gas temperature and ionization can be modelled in the photo-ionization equations. The initial dust distribution and properties can then be self-consistently modified during the RT.

While the currently implemented dust treatment is very simple in that it only accounts for dust absorption (i.e. removal of photons from the ionizing flux by dust), the above considerations were kept in mind during the development, so that introducing a more refined dust modelling is relatively easy in the present code framework.

We created a new software module to include dust following the standard CRASH framework: the dust module is configurable by an ASCII text file, which is loaded along the already existing configuration files for other modules. The file specifies what dust species are considered and from where to load the tables with their optical properties and other dust-related ICs. These are appended to the list presented in § 2:

(vi) dust mass density \( \rho_d \) [g cm\(^{-3}\)];
(vii) fraction of mass \( y_k \) in each dust species \( k \).

To switch between different models, only a configuration change is required, as model-specific values are loaded from files during simulation initialization.

A FORTRAN TYPE DUST\_SPECIES has been created to represent a single dust species and to hold the tables provided by the adopted model. The 3D variability of dust in the computational domain is described with a map of DUST\_IN\_CELL TYPE variables holding the mass density of dust \( \rho_d \), the species mass fractions \( y_k \) and the absorption cross section per mass \( \sigma_d(\nu)/m_d \) in a single cell. According to the frequency sampling adopted in the CRASH spectra, the absorption cross section is computed at each centre-bin frequency \( \nu \) by taking the mass fraction weighted average of the species cross sections:

\[
\frac{d\sigma_d(\nu)}{dm_d} = \sum_k y_k \frac{d\sigma_{d,k}(\nu)}{dm_{d,k}}.
\]

These can be obtained by interpolation of the DUST\_SPECIES tables during CRASH initialization to avoid impacting algorithm performance during photon propagation.

When a photon packet crosses a cell, we account for dust absorption by adding a new term to the optical depth \( \tau_\nu \) from equation (2):

\[
\tau'_\nu = \tau_\nu + \rho_d \frac{d\sigma_d(\nu)}{dm_d},
\]

with the dust mass density \( \rho_d \) in the cell. Equation (4) thus becomes:

\[
\Delta N_{i,\nu} = \frac{\tau'_\nu}{\tau_\nu} \Delta N_\nu.
\]

where \( i \), as before, labels the gas components. The photons absorbed by dust are simply removed from the flux; they do not affect the dust status in any way, i.e. its contribution to the optical depth of the cell stays constant in time. This is, naturally, a point to be improved upon in the future by taking into account radiation processes that modify dust properties and by including the gas to dust coupling they introduce. Photoemission of electrons from grains, for example, is already being implemented and will be included in a future version.

Apart from the modifications discussed here, the RT proceeds as in § 2; specifically the gas ionization equations have not been modified.

5 RESULTS

In this section we present the results of RT simulations in different idealized environments: a dusty H\(_{\text{II}}\) region created by an O-type star (§ 5.1) and a small, cubic cosmological volume with an edge length of 0.5h\(^{-1}\)cMpc in which a few bright stellar type sources propagate their ionizing radiation through dust-enriched gas. The latter test case (§ 5.2) is an adapted version of Test 4 introduced in Iliev et al. (2006) and further discussed in Graziani et al. (2013).

The purpose of these simulations is to verify that our code produces sensible results in simplified configurations mimicking different astrophysical environments in which dust is directly observed (e.g. galactic H\(_{\text{II}}\) regions) or its existence is inferred (e.g. high-z cosmic webs).

Hereafter, the gas is always assumed to be composed of 92\% H and 8\% He by number. At the beginning of any simulation the gas is assumed to be fully neutral and to have a temperature of 100 K. In simulations featuring dust, we assume the dust composition to be the same throughout the entire simulated volume and time.

5.1 Dusty, stellar-type H\(_{\text{II}}\) regions

The configuration we study here oversimplifies the typically clumpy, chemically diverse, dynamic and turbulent star forming environment, by making the following assumptions\(^{10}\):

- The cubic simulation volume of (85 pc\(^3\))\(^3\) contains homogeneous and static gas with a number density \( n_{\text{gas}} = 1 \text{ cm}^{-3} \). This value is typical of the diffuse ionized medium and should be appropriate for an evolved, low-density H\(_{\text{II}}\) region (e.g. Anantharamaih 1986; Roshi & Anantharamaih 2000). The Cartesian grid mapping the volume has a resolution of \( N_C = 256 \) cells per side, corresponding to a spatial resolution of roughly 0.3 pc.
- We pollute the medium with dust using a fixed GDR. Our reference value is GDR = 124, as proposed by WD01 and LD01 for the diffuse ISM. We also explore cases with GDR = 50 and 1000. Similarly, we adopt \( R_V = 3.1 \) in the

\(^{10}\) It should be noted that the problem of the expansion of dusty H\(_{\text{II}}\) regions is far more complicated as dust efficiently couples with radiation, correlating the hydro-dynamics with the RT (e.g. Faucher-Giguère & Quataert 2012; Paladin et al. 2012; Akimkin et al. 2015, 2017). Self-consistent modelling of this problem is beyond the scope of the current work.
reference case and explore models with $R_{V} = 4.0$ and 5.5 (cf. Fig 1).

- The O-type star is modelled as an ideal black-body source\(^\text{11}\) with spectral temperature $T_{BB} = 4 \times 10^{4}$ K and emission rate of ionizing photons $N = 10^{49}$ s\(^{-1}\). These values are appropriate for a powerful O-star (Martins et al. 2006). The source spectrum spans the energy range (13.6–160) eV and it is discretised into $N_I = 67$ frequency bins with adaptive spacing chosen such as to ensure good sampling of the relevant cross sections (cf. Fig. 2). We use $2 \times 10^{8}$ photon packets to sample the source emission. Such a high number is necessary to reach convergence, since especially the dust free and the GDR = 1000 cases proved to be very sensitive to Monte Carlo noise.

- As the lifetime of a massive O-type star ($\lesssim 10$ Myr, e.g. Raiteri et al. 1996) is typically much longer than the ideal ionization timescale for a Strömgren sphere (Draine 2011a, Eq. (15.6)), the H\(^{\text{II}}\) regions observed in our Galaxy are often assumed to be in equilibrium. We run our simulations for $t_{t} = 10$ Myr and find that ionization equilibrium (in H and He) is reached after approximately 1 Myr\(^\text{12}\), while temperature equilibrium is only reached towards the end of the simulations.

Fig. 4 shows spherical averages of hydrogen and helium ionization fractions as well as gas temperature as functions of distance $r$ from the stellar source. All lines show results at the final simulation time $t_{t}$, but correspond to different values of GDR and/or dust models. For comparison we also show the dust-free case. Moreover, we define, somewhat arbitrarily, the radius of the ionization front (I-front) as the one at which $x_{H^{\text{II}}}$ drops below 0.9.

First note that, in absence of dust, CRASH computes an I-front position at radius $r \sim 64$ pc. When the medium is polluted by dust using our reference values (dashed red line), the I-front recedes by $\sim 4$ pc (or 6\%) due to the additional contribution to the total optical depth. Also note that homogeneously distributed dust does not change the slope of the ionization front, which maintains its sharp transition to neutral gas. The increase in optical depth naturally depends on the value of GDR and on the model assumptions leading to variations in the corresponding cross section (see Fig. 1). Changing $R_{V}$ at constant GDR, for example, produces small displacements consistent with the lowering of the dust cross section with increasing $R_{V}$ value. In Appendix A we compare our code to the analytic solution for $x_{H^{\text{II}}}(r)$ by Petrosian et al. (1972).

Close to the source helium is doubly ionized, and $x_{\text{He}^{\text{II}}}$ is correspondingly smaller than unity. Absorption by dust does not have a strong effect on the helium ionization fractions inside the H\(^{\text{II}}\) region until the GDR value is decreased below 100, at which point also the He\(^{\text{II}}\) front begins to recede. This is due to the dust cross section being a factor of two or three larger at H\(^{-}\)-ionizing energies than at He\(^{-}\)-ionizing energies\(^\text{13}\).

The gas temperature profile (bottom panel) reaches values around $T \sim 10^{4}$ K where hydrogen is ionized and quickly drops in the neutral region. Helium provides some additional heating close to the source. As in the case of $x_{H^{\text{II}}}$, absorption by dust reduces the radius of the heated bubble but does not change the structure in the inner region.

In Fig. 5, using the same layout as that of Fig. 4, we show the results of exploring different values of the gas number density $n_{\text{gas}}$ and source ionizing power (i.e. emissivity $\dot{N}$ inside the H\(^{\text{II}}\) region until the GDR value is decreased below 100, at which point also the He\(^{\text{II}}\) front begins to recede.

\(^\text{11}\) While in CRASH arbitrary spectra can be assigned to sources and using a realistic spectrum from a stellar atmosphere model is straightforward, here we opted against this choice as results with an idealized spectrum are of easier interpretation and because the main aim of this test case is to investigate the impact of dust and not to compare our results to observations.

\(^\text{12}\) To reach equilibrium, time dependent RT codes require several ideal ionization times ($\sim 10^{5}$ yr in this case), as simple analytic estimates of such timescales do not account for recombinations that have to be balanced by the ionizing source (e.g. Iliev et al. 2006).

\(^\text{13}\) We find that when the H\(^{\text{II}}\) and He\(^{\text{II}}\) fronts coincide in the dust free medium, as is the case for very hot black-body spectra (cf. Draine 2011a, Ch. 15), they recede jointly in dust polluted media.
and black-body temperature $T_{bb}$), but keeping GDR = 124 (dashed lines). The values chosen for $T_{bb}$ and $N$ are the highest mentioned in Martins et al. (2005, Table 1) for solar metallicity O V stars. For each simulation we also show the corresponding dust free results (solid lines). Our goal here is to obtain a feeling for the possible variation in size of dusty H II regions as predicted by our code.

By increasing the gas number density to $10^4$ cm$^{-3}$ and $10^5$ cm$^{-3}$, the front recedes to 12 pc and 2 pc, respectively, compared to 64 pc for our reference run. The helium ionization regions show the expected behaviour, increasing in size with decreasing density/increasing emissivity and vice versa. Note in the bottom panel that the temperature close to the source is predicted to be higher for weaker sources/higher gas density. This is clearly unphysical and it is owed to the fact that for consistency we used the same spatial resolution of 0.3 pc for all simulations. When we choose more appropriate resolutions to resolve the smaller Strömgren spheres produced at higher densities, this problem is resolved (see inset in last panel).

The effect of dust absorption, again, consists in reducing the size of the ionized regions, while leaving their inner structure unchanged.

We also briefly discuss the effect of dust on ionization fronts in media of lower densities ($n_{gas} \sim 10^{-3}$ cm$^{-3}$), such as the diffuse IGM. Since photon mean free paths are relatively long, transitions from ionized to neutral gas tend to be more extended and feature long low-ionization tails in these cases. We find that the primary effect of dust pollution then is the cut-off of these tails and that only low values of GDR result in a size reduction of the highly ionized region. This effect can also be seen in the simulations we discuss in § 5.2.

Hunt & Hirashita (2009) and Draine (2011b) compiled several observational data sets of galactic and extra-galactic H II regions. Hunt & Hirashita (2009) interpret the observed size-density relation in terms of dynamical semi-analytic models including dust absorption and featuring time dependent $N$. Starting from different initial densities they account for H II region expansion, but retain the assumption of a homogeneous medium. Draine (2011b), on the other hand, interprets the observations in terms of static models that account for radiation pressure on dust creating central densities lower than those close to the ionization front. Our model equilibrium H II regions are too small for a given density, even in dust free cases, to agree with the observational results. This might indicate that our values for $N$ are too low (cf. Hunt & Hirashita 2009, § 4.4), or that the assumption of a homogeneous medium should be removed by accounting for spatial variations of gas density or clumpiness of dust polluted regions. A detailed comparison of these models to our code could provide interesting insights but would go beyond the scope of this paper.

After discussing the equilibrium configurations found in our simulations, we now go over to investigating the effect of dust on the time evolution of H II regions. Fig. 6 shows the growth in time of the ionized bubble at different GDR values, and Fig. 7 shows the expansion speed of the corresponding ionization fronts as a function of time. While initially all fronts coincide and propagate at the same speed, slowdown, dropout and stagnation of fronts in the order of increasing GDR value can be observed at later times when the photons have to traverse a considerable dust column in order to reach the front. The slowdown due to dust absorption might have implications for the overlap of ionized bubbles and consequently for the percolation of dusty media containing several sources (see also § 5.2). Note that we lack the numerical precision to accurately compute speeds lower than $\sim 10$ km/s and that we attribute the premature speed drop in the dust free case to this fact.

A word of caution concerning all above findings is necessary at this point, since our limited dust implementation is, for the time being, not directly coupled to the gas. We work on implementing also grain charging, which results in grains and gas sharing the free electron population\textsuperscript{14}; this

\textsuperscript{14} Note that in general dust will not significantly impact the free electron density in ionized regions, since there is far more mass (and therefore electrons to be released) in the gas than in the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{As Fig. 4 but showing results of simulations varying the gas number density and source ionization power; $(n_{gas}, N, T_{bb}) = (10^{-3}$ cm$^{-3}$, $10^4$ s$^{-1}$, $4 \times 10^4$ K) in green, $(100$ cm$^{-3}$, $10^8$ s$^{-1}$, $4 \times 10^4$ K) in light blue, and $(1$ cm$^{-3}$, $4.3 \times 10^9$ s$^{-1}$, $4.4 \times 10^4$ K) in blue. Dashed lines refer to simulations with GDR = 124, while solid lines correspond to results for dust free media. In the bottom panel we show the temperature profile close to the source for high resolution runs; see text for details. A colour version of this figure is available in the online journal.}
\end{figure}
will introduce direct feedback of dust on gas recombination and cooling, since energetic photo-electrons released from the grains will provide an additional channel for the radiation field to heat the gas. Whether grains provide net heating or cooling thus likely depends on the specific environment being considered (e.g. Weingartner & Draine 2001a) and is one the questions we will investigate in future work. Many other aspects of dust physics can later also be included in the code.

5.1.1 The impact of PAHs

In this section we quantify the impact of PAH removal on the ideal H\textsc{ii} region size of our simple model. Ideally, one should couple the evolution of the PAH population to the RT in time by directly implementing PAH destruction and creation processes in the gas chemistry. However, here we take a far simpler approach and compare simulation runs adopting mixtures with and without PAHs to assess the maximum possible effect on the spherical H\textsc{ii} profiles at equilibrium time.

After verifying that the small differences introduced in the cross sections we computed (see solid black versus dust. In photon-dominated regions, on the other hand, gas-dust reactions can change the electron density (Abel et al. 2008).

Figure 6. Spherical averages of $x_{H\textsc{ii}}$ as function of distance from the black-body source for the dust free case and GDR values 50 and 124 at simulation times $10^3$ yr (upper panel), $10^5$ yr (middle) and $10^7$ yr (lower).

Figure 7. Expansion speed of the H\textsc{ii} ionization front as a function of simulation time for the dust free case and GDR values 50 and 124.

Figure 8. As Fig. 4, but showing results including (excluding) the PAH contribution to the cross section for GDR = 124 in dashed red (dash-dash-dotted cyan) and for GDR = 50 in dotted blue (long dashed orange). For reference, we also show the dust free case (solid black).
dashed red lines in Fig. 3) reproduce the profiles obtained using the Silicate-Graphite-PAH model, we discuss the effects of removing the PAH component (in the bc = 0.0 ppm approach) in Fig. 8 using the example of our reference case (GDR = 124) and the case of GDR = 50.

In our reference case, the effect of the PAH component can be appreciated only in the I-fronts of the hydrogen and temperature profiles, which lie between the full dust and no dust cases as expected, while it is completely negligible in the ionization fractions of helium. This is in line with the finding from the previous section that dust absorption leaves the inner structure of ionized regions unchanged and only affects their fronts. It is thus interesting, albeit purely coincidental, to note that in the GDR = 50 case, the removal of the PAH component nullifies the effects of the dust in the HeII profile, while it provides almost identical fronts to the full dust GDR = 124 case in both hydrogen and temperature profiles.

We also tested the PAH impact on the I-front velocity profiles of the HeII region, finding that in the GDR = 124 case the absence of the PAH component results in a front speed equivalent to the dust free case (black line in Fig. 7). For GDR = 50, instead, the front expands at a rate similar to that of full dust GDR = 124 case.

We have verified that the above conclusions hold qualitatively also if the source has a black body spectral distribution peaking at ~ 17 eV, where PAHs provide the highest absorption, finding no evidence for a strong dependence of our results on the spectral shape.

The impact of the PAH component will be explored again in § 5.2 to investigate a more complex scenario involving a realistic cosmic web and a combination of sources.

### 5.2 RT through a dusty cosmological volume

Here we examine the combined effect of several stellar-type sources on a small cosmic web artificially polluted with dust. This allows us to investigate if a diffuse dusty medium can affect the global pattern of overlapping HII regions with respect to a dust free medium and thus change the morphology and timing of the resulting small scale reionization driven by galactic sources.

To mimic the above process, we adopt the simulation set-up of Test 4 of the Cosmological Radiative Transfer Comparison Project (Iliev et al. 2006), which was later adapted by Graziani et al. (2013) to investigate the effects of atomic-metal pollution. We only briefly describe the RT configuration here and refer to the original papers for more details. The simulation has a box size $L_b = 0.5h^{-1}$ cMpc ($h = 0.72$), a grid resolution $N_c = 128$ (corresponding to a spatial resolution of $4h^{-1}$ ckpc), a volume-averaged gas density $\langle n_{\text{gas}} \rangle = 2.3 \times 10^{-4}$ cm$^{-3}$ and $t_\text{i} = 0.5$ Myr starting at redshift $z = 9$. The cosmological density evolution is not accounted for. 16 hard ($T_{\text{bb}} = 10^5$ K) black-body type sources with emissivities $\dot{N} \sim 10^{52}$ s$^{-1}$ are distributed throughout the volume, and their spectra are sampled using 21 frequencies. $10^8$ photon packets are emitted per source, resulting in sub-permille variations of volume averages when compared to test runs with $2 \times 10^9$ packets.

The gas number density in a slice cut of the simulation volume is shown in Fig. 9. The plane of the slice cut has been selected to intercept one of the most luminous sources as also done in Graziani et al. (2013).

We pollute the medium with dust by simply scaling the gas mass in each cell with a GDR of 124. Note that this, though guided by literature results, is an essentially arbitrary choice, since the abundance of dust at $z = 9$ is observationally unconstrained. Moreover, the restrictions concerning dust evolution and its consequences on extinction as discussed in § 3.2 apply. Our simulation can therefore only give first qualitative results assuming early and efficient dust pollution, which is not inconceivable at this scale. To emulate a decrease of GDR with increasing distance from galactic centres (e.g. Giannetti et al. 2017), we also perform a test using overdensity ($\Delta = n_{\text{gas}}/\langle n_{\text{gas}} \rangle$) dependent GDRs. We find that the tests shown in the following remain largely unaffected when using GDR = 124 in cells with $\Delta > 100$, GDR = 500 for $10 < \Delta < 100$ and GDR = 1000 ($10^5$) in all other cells, even though doing so decreases the total dust mass in the simulation volume to ~ 15% (~ 5%) with respect to the constant GDR case. In future studies we plan to investigate initial conditions generated by hydrodynamic simulations that treat dust in a self-consistent manner. Dust abundances are, however, also highly uncertain from a theoretical/numerical point of view, especially on the circumgalactic medium scale, where they strongly depend on the feedback model adopted in a simulation.

In Fig. 10 we present contour maps of the plane shown in Fig. 9 at the time $t = 5 \times 10^4$ yr, comparing results obtained without dust (left), with the full dust mixture (middle) and with PAH free dust (right). The volume averaged H ionization fractions are 0.14, 0.12 and 0.13, respectively. First note that, owed to the shape of the spectrum of the sources, HeII regions tend to be more extended than HII regions (see also Graziani et al. 2013, Fig. 3 and § 5.2.3). Moreover, it is difficult to investigate the shape of a single ionized region as there are multiple sources in the main over-dense filament seen in Fig. 9, and at the chosen time several ionized bubbles already overlap. In the top panels, where
ionized hydrogen is shown, we immediately note the sharpening of ionization fronts. The degree of \( \text{H} \text{II} \) region overlap is consequently reduced by the presence of dust, changing the spatial distribution of the ionized regions in the polluted medium. An even more pronounced effect is visible in the \( x_{\text{He} \text{II}} \) and \( x_{\text{He} \text{III}} \) patterns, where the ionizing flux subtracted by the dust also favours a faster helium recombination. In the bottom panel, the gas temperature distribution is shown. The indirect effects of dust absorption on the gas temperature are evident in the form of a less progressive transition between cold (\( T \sim 10^2 \) K) and hot (\( T \sim 10^4 \) K) gas.

We call particular attention to two points: first, note how at coordinates \((45 \, \text{kpc}, 45 \, \text{kpc})\) in the second row the highly ionized regions overlap in the dust free case, whereas they hardly touch in the dust polluted case. Second, one can appreciate at \((40 \, \text{kpc}, 35 \, \text{kpc})\) how self-shielding neutral pockets can survive longer in the presence of dust.

The effects of removing the PAH component correspond to what one would expect from our study of single \( \text{H} \text{II} \) regions, i.e. without PAHs the I-fronts fall between those of the dust free and full dust cases. We do therefore not discuss the right column in more detail.

Fig. 11 gives a quantitative view of the differences between our dust free, dust polluted and PAH free results. It shows the distribution of all cells in the simulation volume at \( t = 5 \times 10^4 \) yr for \( x_{\text{H} \text{II}}, x_{\text{He} \text{II}}, x_{\text{He} \text{III}} \) and \( T \). As one would expect from the above discussion, dust increases the number of neutral cells, reduces the amount of weakly ionized cells and leaves the number of highly ionized cells nearly unchanged. Moreover, it shifts the peak corresponding to hot, ionized cells in the temperature distribution towards lower temperatures and reduces the amount of cells heated to \( \sim 10^3 - 3 \times 10^4 \) K.

Owed to the location of the peak of dust absorption,
$x_{\text{He} \text{II}}$ and $T$ are most affected in volume averages. In Fig. 12 we therefore show the corresponding time evolution. At 0.2 Myr, the dust free case has a volume averaged $x_{\text{He} \text{II}}(T)$ of 0.54 (3.2 $\times 10^4$ K), which is reduced by 20% (25%) in the full dust case and 12% (16%) in the PAH free case.

To investigate the dependence on the spectral shape of all the above findings, we performed simulation runs in which we used $T_{\text{bb}} = 4 \times 10^4$ K black-body spectra for the sources, while keeping all the other parameters fixed. The associated shift in the spectrum peak primarily results in less helium ionization and in a lower average gas temperature, but qualitatively the above observations still hold.

Dust can offer significant absorption at ionizing energies. The simple cases studied here show sensitive alterations of size, shape and time evolution of ionized regions: ionization fronts get sharpened, the size of fully ionized regions is reduced changing their degree of overlap and the gas temperature is lowered. These effects can certainly have a strong impact on small scale RT simulations, where dust is known to be present and its spatial extent can be resolved. It should be considered, however, that other physical processes currently not included in our implementation can be important. In particular, dust photo-heating is likely to have a strong impact on the gas temperature and will have to be accounted for in the future. Further observational and numerical investigations of the spatial distribution, abundance and chemical properties of dust are required in order to critically examine the assumptions made, to determine the appropriate physical set-up of future RT simulations and to precisely quantify the impact of absorbing grains on the final ionization and temperature patterns created in the many different environments of both the ISM and the IGM.

6 CONCLUSIONS

In this work we have extended the Monte Carlo Radiative Transfer (RT) code for ionizing ($\nu \geq 13.6$ eV) radiation CRASH by a dust module that, at the moment, accounts for the absorption of radiation by dust. We have used this new implementation to study the formation of idealized H II regions by point-like stellar sources and found that including dust leaves their inner ionization and temperature structure largely unchanged. As expected (e.g. Draine 2011a), however, it can result in a significant reduction in size. For monochromatic sources, our code predicts H II region sizes in accordance with semi-analytic solutions (see Appendix A). Furthermore, we have performed a first step towards investigating the effect of dust on small scale reionization by performing RT on a small cosmological volume artificially polluted with dust and containing several black-body sources. Here we find that dust primarily sharpens ionization fronts and slows down the overlap of intergalactic ionized bubbles. This, naturally, also results in a decrease in volume of hot ($\sim 10^4$ K) gas. There seems to be only a weak dependence of these results on the gas-to-dust mass ratio used in the underdense regions of the cosmological volume.

The next project we plan to approach using the implementation presented here is investigating non-equilibrium ionization by Active Galactic Nuclei (AGN), complementing the work done in Kakiichi et al. (2017) with dust. Such sources allow studying X-ray effects since they emit large numbers of photons at high energies, where the dust cross section gains importance in comparison with the gas cross section. In the future we plan to simulate RT in post-processing on gas and dust distributions self-consistently computed by hydrodynamics codes. This is a crucial step to improve on the simple dust distributions used here. Moreover, the dust physics in our model will be further developed to include effects such as grain charging, heating and destruction.

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Figure 11. Distributions of all cells in the simulation volume in (left to right) $x_{\text{H}^{\text{ii}}}$, $x_{\text{He}^{\text{ii}}}$, $x_{\text{He}^{\text{iii}}}$ and $T$ at $t = 5 \times 10^4$ yr for the dust free (solid black line), dust polluted (dashed red) and PAH free (dotted blue) runs. The cells were distributed onto 200 bins.

Figure 12. Time evolution of the volume averaged $x_{\text{He}^{\text{ii}}}$ (top panel) and $T$ (bottom) for our dust free (solid black line), GDR = 124 (dashed red) and PAH free (dotted blue) run.

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In Fig. A1 we show $x_{\text{HI}}$ as computed by CRASH (solid lines) as well as the corresponding solutions of the numerical integration (dashed lines) as discussed in Raga & Lora (2015). The simulations shown in this figure are set up as described in §5.1, with $n_{\text{gas}} = 1 \text{ cm}^{-3}$ and various GDR values. For a meaningful comparison, we have made the following changes:

- He abundance is set to zero;
- the source emits monochromatic photons at $13.6 \text{ eV}$;
- the gas temperature is set to $T = 10^4 \text{ K}$ in the entire simulation volume and kept constant during the simulation; and
- case B recombination is enabled.

Note that there is a typo in Eq. (7) of the paper. $1 - y^{3/4}$ should read $1 - y^{3/4}$.
As our scheme is time dependent, we must compare the ionization structure obtained once an equilibrium configuration is reached to a solution obtained explicitly assuming equilibrium. Despite this, the agreement of the results is remarkably good in a wide range of gas number densities (due to the limited space available, we do not show the tests performed at number densities other than 1 cm\(^{-3}\) here) and values of GDR. In the cases without dust, GDR = 1000 and 124, the location of the I-front is very well reproduced by CRASH, while intrinsic differences between numerical algorithm and analytic solution can induce a wider/narrower declining front. For GDR = 50, CRASH slightly overpredicts absorption, but remains in good agreement. It should be noted that an exact comparison between (semi-)analytic solutions and predictions of numerical RT codes is always difficult beyond the I-front position for a number of reasons. First, each numerical method has its own intrinsic issues in sampling the radiation field: the long-characteristic method implemented in CRASH, for example, requires a large number of photon packets to correctly cover the small angle of emission of isotropic sources. Without the appropriate angular coverage adopted here and in § 5.2, at large distances from the source the declining fronts would show a spiky behaviour due to the geometrical separation of the few rays escaping the I-front. This computational issue is solved in short-characteristic approaches but at the price of having less radial coherence in the propagating packets. Second, and more important, analytic solutions often rely on over-simplifications that advanced numerical codes have been build to encompass (e.g. single frequency photons, fixed temperature, missing collisional/secondary ionization, etc.). The collisional ionization term, for example, is generally neglected in the analytic estimates while fully implemented in CRASH as function of the evolving temperature and cannot be switched off during the simulation. Depending on the assumed gas density and temperature this term could induce significant differences in the way the ionization fronts decline at imposed, constant temperature. Finally, note that apart from these idealized set-ups, all the simulations shown in this paper adopt consistent temperature and ionization computations as well as appropriate numbers of photons packets to satisfy Monte Carlo convergence of the results and to minimize the intrinsic numerical noise mentioned above.

From further tests we conducted following the above findings, we conclude that for \(n_{\text{gas}} \leq 1 \text{ cm}^{-3}\) and GDR \(\geq 50\), and for \(n_{\text{gas}} \leq 0.1 \text{ cm}^{-3}\) and GDR \(\geq 10\) our scheme shows good agreement with the numerical integration, while caution should be exercised for higher gas and dust densities. In those regimes the time independent dust optical depth significantly alters the time evolution of the I-front and reduces its final equilibrium radius by up to a factor of a few with respect to the numerical integration. We are further investigating this and believe careful comparisons with other time dependent RT schemes accounting for dust would provide helpful insights.

**APPENDIX B: MODELING THE EFFECT OF PAH DESTRUCTION ON THE DUST CROSS SECTION**

Since no full model of the processing of PAHs in H\(\text{II}\) regions is available, it is not clear how one should modify a given grain size distribution and thus the resulting cross section (see § 3.3) of a dust mixture to account for it. We explore three different approaches here, presented in detail in the following. Note that we never change the distribution of silicate grains.

As described in § 3.2, the Silicate-Graphite-PAH model does not feature a separate PAH population, but PAHs are rather modelled as a part of the carbonaceous grain population. Specifically, LD01 introduce in Eq. (3) a PAH “weight” \(\xi_{\text{PAH}}(a)\), where \(a\) is the effective grain radius, which they use to make a transition from graphite to PAHs in the absorption cross section of carbon grains (see Eq. (2) of LD01). The total optical depth per distance \(l\) due to carbon dust with cross section \(\sigma_{\text{carb}}(a,\nu)\) and grain size distribution \(d\sigma_{\text{carb}}/da\) is then computed as:

\[
\frac{\tau_{\text{carb}}(\nu)}{l} = \int da \frac{d\sigma_{\text{carb}}}{da} \sigma_{\text{carb}}(a,\nu) = \int da \frac{d\sigma_{\text{carb}}}{da} (\xi_{\text{PAH}}\sigma_{\text{PAH}}(a,\nu) + (1 - \xi_{\text{PAH}})\sigma_{\text{gra}}(a,\nu)),
\]

with PAH \((\sigma_{\text{PAH}}(a,\nu))\) and graphite \((\sigma_{\text{gra}}(a,\nu))\) cross sections as defined in WD01.

In our first approach, which we refer to as “split”, we propose to split the carbon grain population into a PAH and a graphite population, i.e. we define grain size distributions

\[
\frac{d\sigma_{\text{PAH}}}{da} = \xi_{\text{PAH}}(a) \frac{d\sigma_{\text{carb}}}{da}
\]

and

\[
\frac{d\sigma_{\text{gra}}}{da} = (1 - \xi_{\text{PAH}}(a)) \frac{d\sigma_{\text{carb}}}{da}.
\]

With these definitions, the total carbon dust optical depth becomes:

\[
\frac{\tau_{\text{carb}}(\nu)}{l} = \int da \left( \frac{d\sigma_{\text{PAH}}}{da} \sigma_{\text{PAH}}(a,\nu) + \frac{d\sigma_{\text{gra}}}{da} \sigma_{\text{gra}}(a,\nu) \right) = \frac{\tau_{\text{PAH}}(\nu)}{l} + \frac{\tau_{\text{gra}}(\nu)}{l}.
\]

To account for H\(\text{II}\) region processing, we then set \(d\sigma_{\text{PAH}}/da\) to zero when computing cross sections.

The motivation for this approach lies in excluding the contribution to the cross section attributed to PAHs in the Silicate-Graphite-PAH model. This does, however, result in a size distribution (see dashed red line in Fig. B1) unlikely to represent physical reality, since it features a kink at 50 Å and rises again towards the lower size limit, while the smallest PAHs are expected to be the most susceptible to photodissociation (e.g. Bocchio et al. 2012).

Draine & Li (2007) use \(q_{\text{PAH}}\), the mass fraction of dust contained in carbonaceous particles with fewer than 1000 C atoms, to quantify the PAH content of a given grain size distribution. Although the PAH destruction efficiency is unlikely to feature a sharp transition specifically at 1000 C
atoms (roughly 13 Å in effective radius), we base our second approach, referred to as “cut” (dotted blue line in Fig. B1), on this definition and sharply cut the carbon grain size distribution here when computing cross sections for H II region processed dust. Otherwise the carbon grains are treated as in the original model.

In the third approach we set $b_C = 0.0$ ppm while keeping all other parameters of the size distributions fixed. This removes the two log-normal distributions that WD01 add to the power-law distribution for the carbonaceous grain population, significantly reducing the number of small carbon grains. We then proceed as in the cut case described above. This approach is motivated by the fact that the MW3.1L00 model from WD01 (see also Draine & Li 2007, Table 3), which also does not include log-normal distributions, is used to fit dust emission from regions of expected low PAH content (Draine & Li 2007; Chastenet et al., in prep.). It produces the most plausible distribution (dash-dotted orange line) and predicts essentially the same cross section as our split approach (see Fig. 3).

To explore the effect of our modified grain size distributions, knowledge of the absorption cross section as a function of photon energy and grain size is required. We can therefore not rely on the published tables of population-averaged cross sections as in the main text of the paper. Instead, we follow the prescriptions given in WD01, LD01 and Draine (2003a,b,c) to directly compute cross sections. Although we plan to investigate the transfer of X-rays in the future, for the purposes of this paper we can restrict our attention to the energy range 13.6–160 eV, since none of the spectra we used here extends beyond this range. As stated in § 3 of Draine (2003c), the Wiscombe Mie theory code was used to compute graphite and silicate cross sections for $x = 2\pi a / \lambda < 2 \times 10^4$, with $\lambda$ the photon wavelength. For $h\nu = 160$ eV and $a = 10$ µm (upper limit of the grain size distribution), $x \approx 8100$, so that we use Mie theory\(^\text{16}\) in the entire energy range. For the PAH cross section we use Eqs. (5) to (11) from LD01, although only Eqs. (5), (6) and (7) are relevant for our energy range. Note that in this regime the cross sections of neutral and ionized PAHs are identical. Cross sections for energies up to ~31 eV as a function of grain size are also provided by DustEM (Compiègne et al. 2010) in pre-computed tables, which can alternatively be used as input for our framework. We verified that using these data gives results in good agreement with those from the direct Mie computation. The framework used for these computations will be made publicly available on GitHub.

This paper has been typeset from a TeX/LaTeX file prepared by the author.

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\(^{16}\) We obtained a version of the Wiscombe code at scatterlib.wikidot.com/mie and downloaded Draine (2003b) dielectric functions from astro.princeton.edu/~draine/dust/dust.diel.html.