Ionization feedback in star formation simulations: the role of diffuse fields

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ABSTRACT
We compare the three-dimensional gas temperature distributions obtained by a dedicated radiative transfer and photoionization code, MOCASSIN, against those obtained by the recently developed smooth particle hydrodynamics (SPH) plus ionization code iVINE for snapshots of a hydrodynamical simulation of a turbulent interstellar medium (ISM) irradiated by a nearby O star. Our tests demonstrate that the global ionization properties of the region are correctly reproduced by iVINE, hence validating further application of this code to the study of feedback in star-forming regions. However, we highlight potentially important discrepancies in the detailed temperature distribution. In particular, we show that in the case of highly inhomogeneous density distributions, the commonly employed on-the-spot (OTS) approximation yields unrealistically sharp shadow regions which can affect the dynamical evolution of the system. We implement a simple strategy to include the effects of the diffuse field in future calculations, which makes use of physically motivated temperature calibrations of the diffuse-field-dominated regions and can be readily applied to similar codes. We find that while the global qualitative behaviour of the system is captured by simulations with the OTS approximation, the inclusion of the diffuse field in iVINE (called D\textsc{-}iVINE) results in a stronger confinement of the cold gas, leading to denser and less coherent structures. This in turn leads to earlier triggering of star formation. We confirm that turbulence is being driven in simulations that include the diffuse field, but the efficiency is slightly lower than in simulations that use the OTS approximation.

Key words: radiative transfer – turbulence – stars: formation – ISM: structure.

1 INTRODUCTION

Ionizing radiation from OB stars influences the surrounding interstellar medium (ISM) on parsec scales. As the gas surrounding a high-mass star is heated, it expands forming a H\textsc{ii} region. The consequence of this expansion is twofold: first, gas is removed from the centre of the potential, preventing it from further gravitational collapse. Secondly, gas is swept up and compressed beyond the ionization front, producing high-density regions that may thus be susceptible to gravitational collapse (i.e. the ‘collect and collapse’ model; Elmegreen, Kimura & Tosa 1995). Furthermore, pre-existing, marginally gravitationally stable, clouds may also be driven to collapse by the advancing ionization front (i.e. ‘radiation-driven implosion’; Bertoldi 1989; Kessel-Deynet & Burkert 2003; Gritschneder et al. 2009a). Finally, ionization feedback is also thought to be a driver for small-scale turbulence in a cloud (Gritschneder et al. 2009b, hereafter G09b). The net effect of photoionization (PI) feedback on the global star formation efficiency is still, however, under debate.

While the importance of studying the PI process as part of hydrodynamical star formation simulations has long been widely recognized, until very recently, due to the complexity and computational demand of the problem, the evolution of ionized gas regions had only been studied in rather idealized systems (e.g. Yorke et al. 1989; Garcia-Segura & Franco 1996), with simulations often lacking resolution and dimensions. Fortunately, the situation in the recent years has been rapidly improving, with more sophisticated implementations of ionized radiation in grid-based codes presented by (e.g.) Mellema et al. (2006), Krumholz, Stone & Gardiner (2007) and Peters et al. (2010).

Kessel-Deynet & Burkert (2000) were the first to introduce an ionization algorithm into a smoothed particle hydrodynamical (SPH) code to study radiation-driven implosion as a possible trigger of star formation. Later, Dale, Ercolano & Clarke (2007) presented a much simplified, but fast, algorithm to consider PI within complex
SPH simulations. When compared to grid codes, which are based on the solution of the Eulerian form of the same equations, much higher resolution of very complex flows can be achieved. Since Dale et al. (2007), a number of other ionizing radiation implementations have been developed for SPH codes, including Pawlik & Schaye (2008), Altay, Croft & Pelupessy (2008), Bissas et al. (2009) and very recently Gritschneder et al. (2009a). However, high-resolution SPH simulations are very computationally expensive, and even in the current era of parallel computing, an exact solution of the radiative transfer (RT) and PI problem in three dimensions within SPH calculations is still prohibitive. Necessarily, all the algorithms mentioned above employ an extremely simplified approach to RT and PI. The consequences of such simplification on the conclusions drawn from the simulations need to be investigated.

In Dale et al. (2007), we performed the only such verification to date against a fully three-dimensional RT and PI code (MOCASSIN; Ercolano et al. 2003; Ercolano, Barlow & Storey 2005; Ercolano et al. 2008a) for complex density fields obtained from the SPH calculations. We showed in that case that the agreement on the ionized fractions in high-density regions was very good, but low-density regions were poorly represented by the ionization + SPH code. In this paper, we take a similar approach to test the more recent algorithms developed in iVINE (Gritschneder et al. 2009a). We find excellent agreement between the codes for the global ionization fractions; however we highlight discrepancies in the temperature distribution, particularly in shadow regions that are dominated by the diffuse field, which is not accounted for in iVINE. We test the consequences of the omission of the diffuse field both on the hydrodynamical evolution of the structure and on the evolution of the turbulence spectrum using a simple approach that allows for a more realistic but still efficient modelling strategy of the shadow regions.

In Section 2, we briefly describe the iVINE and MOCASSIN codes and the comparison strategy. In Section 3, we show the results of this comparison. In Section 4, we discuss a simple approach to qualitatively include diffuse-field effects in iVINE and show the results from these further tests in Section 5. Section 6 contains a brief summary and future directions.

2 NUMERICAL METHODS

We have used the MOCASSIN code (Ercolano et al. 2003, 2005, 2008a) to calculate the temperature and ionization structure of the turbulent ISM density fields presented by G09b and Gritschneder et al. (2010). The SPH quantities were obtained with the iVINE code (Gritschneder et al. 2009a) and mapped on to a regular 128^3 Cartesian grid. We briefly describe the set-up of the two codes and summarize the strategy for our comparative tests.

2.1 iVINE

iVINE (Gritschneder et al. 2009a) is a highly efficient fully parallel implementation of ionizing radiation in the tree-SPH code VINE (Nelson, Wetzstein & Naab 2009; Wetzstein et al. 2009). While the treatment of hydrodynamics and gravitational forces is fully three dimensional, the ultraviolet radiation of a massive star is assumed to impinge along parallel rays on to the simulated domain. To keep the computational effort small, the radiation is assumed to be monochromatic. In addition, ionizing photons re-emitted following recombinations are assumed to be immediately absorbed in the direct neighbourhood [on-the-spot (OTS) approximation, e.g. Spitzer 1978]. On the surface of infall, the domain is decomposed into small rays. Along these rays, the radiation is propagated from SPH particle to SPH particle by iterating the ionization degree to its equilibrium value. This is done at the smallest hydrodynamical time-scale, i.e. after each hydrodynamical time-step. The newly found ionization degree $\eta$ is then coupled to the hydrodynamic evolution via the gas pressure of each individual particle $i$:

$$ P_i = \left( \frac{T_{\text{hot}} \eta_i}{\mu_{\text{hot}}} + \frac{T_{\text{cold}}(1 - \eta_i)}{\mu_{\text{cold}}} \right) \frac{k_B \rho_i}{m_p}, $$

where $T_{\text{hot}} = 10 \text{ kK}$ and $T_{\text{cold}} = 10 \text{ K}$, and $\mu_{\text{hot}} = 0.5$ and $\mu_{\text{cold}} = 1.0$ are the temperatures and the mean molecular weights of the ionized and the un-ionized gas, respectively, in the case of pure hydrogen. $k_B$ is the Boltzmann constant, $m_p$ is the proton mass and $\rho_i$ is the SPH density of the particle. To ensure a correct treatment of the newly ionized particles, their time-step is reduced according to the ratio of the sound speeds in the hot and the cold gas. For a detailed description along with numerical tests, see Gritschneder et al. (2009a). The accuracy parameters for the simulations presented here are as given in G09b.

To map the complex particles distribution obtained with the iVINE code on an equally spaced Cartesian grid, we bin the particles weighted with the SPH kernel. For each particle, the grid cells which are inside the particles smoothing length are determined. On to these cells, the mass of the SPH particle is then distributed according to a weight obtained by equating the kernel for the given distance between particle and grid cell. All other quantities are weighted accordingly.

2.2 MOCASSIN

MOCASSIN is a three-dimensional PI and dust RT code that employs a Monte Carlo approach to the frequency-resolved transfer of radiation. The code includes all the dominant microphysical processes that influence the gas ionization balance and the thermal balance of dust and gas, including processes that couple the gas and dust phases. In the case of H II regions ionized by OB stars, the dominant heating process for typical gas abundances is PI of hydrogen, which is balanced by cooling by collisionally excited line emission (dominant), recombination line emission, free–bound and free–free emission. The atomic data base includes opacity data from Verner et al. (1993) and Verner & Yakovlev (1995), energy levels, collision strengths and transition probabilities from Version 5.2 of the CHIANTI database (Landi et al. 2006, and references therein) and the improved hydrogen and helium free–bound continuous emission data of Ercolano & Storey (2006). The code was originally developed for the detailed spectroscopic modelling of ionized gaseous nebulae (e.g. Ercolano et al. 2004, 2007), but is regularly applied to a wide range of astrophysical environments, including protoplanetary discs (e.g. Ercolano et al. 2008b; Ercolano, Clarke & Drake 2009; Owen et al. 2010; Schisano, Ercolano & Güdel 2010) and supernova envelopes (e.g. Sugerman et al. 2006; Ercolano et al. 2007b; Wesson et al. 2008; Andrews et al. 2010). Arbitrary ionizing spectra as well as multiple ionization sources whose ionized volumes may or may not overlap can be used, with the overlap region being self-consistently treated by the code. Arbitrary dust abundances, compositions and size distributions can be used, with independent grain temperatures calculated for individual grain sizes.

In order to compare with iVINE, the stellar field was assumed to be incident along parallel rays, but the subsequent RT was performed in three dimensions, hence allowing for an adequate representation of the diffuse field. We scaled the incoming stellar field to the value used by G09b ($F_{\text{Ly}} = 5 \times 10^5 \text{ photon cm}^{-2} \text{ s}^{-1}$), and we assumed...
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Figure 1. Surface density projected in the \( z \)-direction of the \( t = 9 \) kyr (left-hand panel), 250 kyr (middle panel) and 500 kyr (right-hand panel) snapshots of G09b's turbulent ISM simulation. The upper panels show the evolution of the gas without diffuse field, the lower panels show the same simulation performed with the simplified diffuse-field implementation discussed in Section 4. The white boundaries on the left-hand panels mark the regions compared in Table 1. The SPH particles were mapped on to a \( 128^3 \) regular Cartesian grid.

2.3 Strategy for comparison test

The comparisons are based on the simulations of G09b which address the impact of ionizing radiation on a turbulent ISM. These simulations used \( 2 \times 10^6 \) SPH particles, which are set up to resemble a medium with an average number density of \( 300 \) cm\(^{-3} \) in a volume of \((4 \text{ pc})^3\). To mimic turbulence, a supersonic velocity field with Mach 10 is set up on the largest modes. This set-up is allowed to decay freely down to a turbulent Mach number of 5 before the ionization field is switched on. We have taken snapshots of this simulation at several time-steps and mapped the corresponding SPH particle fields to a \( 128^3 \) Cartesian grid.

We have taken snapshots at several time-steps in the turbulent ISM simulation of G09b and mapped the corresponding SPH particle fields to a \( 128^3 \) Cartesian grid. Fig. 1 shows the surface density projected in the \( z \)-direction for the \( t = 9 \) kyr (left-hand panel), \( t = 250 \) kyr (middle panel) and \( t = 500 \) kyr (right-hand panel) snapshots. The top panels show the results from the original G09b calculation (no diffuse field), while the bottom panels show the same results for the approximate diffuse-field calculation presented in Section 4. The comparison tests discussed in Section 3 were performed using the distributions from the original G09b calculation shown in the top panels.

Three-dimensional RT and PI calculations were performed on the Cartesian grid using MOCASSIN as described above. We run H-only simulations (referred to as ‘H-only’) as well as simulations with typical H\( \text{ II} \) region abundances (referred to as ‘Metals’). The elemental abundances for the metal-rich model were as follows, given as number density with respect to hydrogen: He/H = 0.1, C/H = 2.2\( \times \)10\(-4\), N/H = 4.0\( \times \)10\(-5\), O/H = 3.3\( \times \)10\(-4\), Ne/H = 5.0\( \times \)10\(-5\), S/H = 9.0\( \times \)10\(-6\).

We compared the resulting MOCASSIN temperature and ionization structure grids to \( \text{iVINE} \) with the aim to address the following questions. (i) Are the global ionization fractions accurate? (ii) How accurate is the gas temperature distribution? (iii) What is the effect of the diffuse field? (iv) How can the algorithm be improved?

3 RESULTS

In this section, we present the results of our comparison of the original G09b \( \text{iVINE} \) calculations (top panels in Fig. 1) with MOCASSIN. We limit the discussion to the \( t = 500 \) kyr snapshot, but we note here that the same conclusions apply to the other time-steps (we have performed the same tests at several time snapshots).

3.1 Global properties

Fig. 2 shows the surface density of electrons projected in the \( z \)-direction for the G09b turbulent ISM simulation at \( t = 500 \) kyr. The figure shows that the integrated ionization structure is reasonably well reproduced by \( \text{iVINE} \). There are however some qualitative differences at the rear of the grid (\( X > 3 \) pc) where \( \text{iVINE} \) predicts a lower surface density of electrons (i.e. a more neutral gas). This is due to the fact that these regions are completely shielded from ionizing photons in \( \text{iVINE} \) by overlapping shadows. In the MOCASSIN simulations, however, reprocessed photons are able to diffuse amongst the clumps and reach the rear of the domain. Nevertheless, these differences are small and the global ionization structure is correctly determined by \( \text{iVINE} \), as confirmed by the simple comparison.
of the total ionized mass fractions: at \( t = 500 \text{ kyr} \), \( \dot{\text{VINE}} \) obtains a total ionized mass of 13.9 per cent, while \( \text{MOCASSIN} \) 'H-only' and 'Metals' obtain 15.6 and 14.0 per cent, respectively. The agreement at other time snapshots is equally good (e.g. at \( t = 250 \text{ kyr} \), \( \dot{\text{VINE}} \) obtains 9.1 per cent and \( \text{MOCASSIN} \) 'Metals' 9.5 per cent).

It may at first appear curious that the agreement should be better between \( \dot{\text{VINE}} \) and \( \text{MOCASSIN} \) 'Metals', rather than \( \text{MOCASSIN} \) 'H-only', given that only H ionization is considered in \( \dot{\text{VINE}} \). This is however simply explained by the fact that \( \dot{\text{VINE}} \) adopts an 'ionized gas temperature' (\( T_{\text{hot}} \)) of 10 kK, which is close to a typical \( \text{H} \text{II} \) region temperature, with typical gas abundances. The absence of metals in the \( \text{MOCASSIN} \) 'H-only' simulations causes the temperature to rise to typical values close to 17 kK, due to the fact that cooling becomes much less efficient without collisionally excited lines of oxygen, carbon, etc. The hotter temperatures in the 'H-only' models directly translate into slower recombinations, as the recombination coefficient is roughly proportional to the inverse of the temperature. As a result of slower recombinations the 'H-only' grids have a slightly larger ionization degree.

3.2 Ionization and temperature structure

The gas temperature of a particle in \( \dot{\text{VINE}} \) is calculated as a simple function of the ionization fraction, \( \eta \), i.e.

\[
T_e = T_{\text{hot}} \eta + T_{\text{cold}}(1 - \eta),
\]

(2)

where \( T_{\text{hot}} = 10 \text{kK} \) and \( T_{\text{cold}} = 10 \text{K} \) are the temperatures assigned to fully ionized and neutral material, respectively. Accurate gas temperatures are of prime importance as this is how feedback from ionizing radiation impacts on the hydrodynamics of the system (cf. equation 1). In Fig. 3 we compare the electron temperatures \( T_e \) calculated by \( \dot{\text{VINE}} \) and \( \text{MOCASSIN} \) ('H-only' and 'Metals') in a \( z \)-slice of the \( t = 500 \text{ kyr} \) grid. The top right-hand panel of the figure shows the volumetric number density (cm\(^{-3}\)) map for the selected slice. The large shadow regions behind the high-density clumps in the \( \dot{\text{VINE}} \) calculations are immediately evident in the figure. These shadows are largely reduced in the \( \text{MOCASSIN} \) calculations as a result of diffuse-field ionization. The diffuse field is softer than the stellar field and therefore temperatures in the shadow regions are lower than in the directly illuminated regions. Fig. 4 shows a more quantitative comparison of the temperature distribution along a single ray intercepting a high-density clump and its shadow region. The ray is marked in Fig. 3 as the solid black line in the top left-hand panel. The dashed line in Fig. 4 shows the logarithmic hydrogen number density as a function of distance into the grid. The black solid line is the electron temperature along the ray as determined by \( \dot{\text{VINE}} \), while the solid red and blue lines are the electron temperatures determined by \( \text{MOCASSIN} \) 'H-only' and 'Metals', respectively. The higher temperatures in the shadow regions of the \( \text{MOCASSIN} \) 'Metals' model are a consequence of the helium Lyman radiation and the heavy elements free–bound contribution to the diffuse field.

The effects of radiation hardening and of the recombination of some of the important cooling ions is also apparent in \( \text{MOCASSIN} \)'s temperatures which rise with distance from the star in the directly illuminated regions. As expected, the effect is much more pronounced in the 'Metals' model (a steeper temperature distribution in metal-rich regions is a well-known effect, e.g. Stasińska 2005; Ercolano et al. 2007b). Radiation hardening is accounted for in some 'monochromatic' RT codes by pre-calculating the effective PI x-section as a function of the Lyman-limit optical depth by integrating over the extinguished stellar spectrum and doing the same for the photoelectric heating integral (e.g. c2ray; Mellema et al. 2006). Helium, heavy elements or dust effects are not included by this treatment however and most importantly the effects of different coolants acting in different regions (which is dominating the temperature distribution in the directly illuminated regions of the \( \text{MOCASSIN} \) Metals calculations) cannot be accounted for in this way. In future work, we plan to provide simple temperature calibrations to account for the environmentally driven temperature gradients in the directly illuminated regions. We note however that errors in the temperature of the directly illuminated regions are unlikely to exceed factors of 2 at most, the errors on the temperature of the diffuse-field-dominated regions, on the other hand, are typically 3 orders of magnitude (10 K compared to 10 kK). Thus, in the remainder of this paper we shall focus on the larger temperature differences in the shadowed regions and how they may affect the hydrodynamical evolution of the system.

4 GAS TEMPERATURES IN SHADOW REGIONS

As \( \dot{\text{VINE}} \) solves the transfer along plane-parallel rays using the OTS approximation (e.g. Spitzer 1978; Osterbrock & Ferland 2006), it has currently no means of bringing ionization (and hence heating) to regions that lie behind high-density clumps. This creates sharp shadows with a large temperature (pressure) gradient between neighbouring direct and diffuse-field-dominated regions, which may have
important implications for the dynamics, particularly with respect to turbulence calculations.

In order to explore the significance of the error introduced by the OTS approximation on the dynamics of the system, we propose here a simple strategy to include the effects of the diffuse field in iVINE, which can be readily extended to other similar codes. It can be summarized in the following steps: (i) identify the diffuse-field-dominated regions (shadow); (ii) study the realistic temperature distribution in the shadow region using fully frequency-resolved three-dimensional PI calculations performed with MOCASSIN and parametrize the gas temperature in the shadow regions as a function of (e.g.) gas density and (iii) implement the temperature parametrization in iVINE and update the gas temperatures in the shadow regions at every dynamical time-step accordingly.

In what follows, we describe our zeroth-order implementation of the above strategy for the case at hand, but we stress that this can be adapted to different situations. In future work, we will present a generalized version of the procedure detailed below, which will include temperature parametrizations for both the direct and diffuse-field-dominated regions and will account for different environments and geometrical set-ups of the codes. This requires a parameter space study and is beyond the scope of the current work, where we only aim to assess the relevance of relaxing the OTS approximation for highly inhomogeneous cases.

4.1 Step (i): identify the shadows

In the case of iVINE, we identify the diffuse-field-dominated regions by means of simple criteria that need only be evaluated along a ray, such that no significant overheads are introduced by this step. A particle/grid cell is initially defined to be ‘shadowed’ if iVINE would assign a temperature of $T < 100\,\text{K}$ to it, i.e. if its ionization degree is $\eta < 10^{-2}$.
cells that do not obey equation 2) is more realistically described by photon-dominated region (PDR) conditions, with temperatures closer to 1000 K, rather than 10 K. So the error introduced by applying equation (2) to the true shadow zone in the $10 \text{ cm}^{-3} < n_{\text{H}} < 100 \text{ cm}^{-3}$ range is still smaller than if those cells had been assigned their original temperature of 10 K.

A second-order problem is posed by the large scatter of the data (red points) shown in Fig. 5. Typical errors of $\sim$50 per cent in temperature are to be expected with this method. The temperature at a given location in an ionized region is expected to roughly scale with the local ionization parameter, which is defined as the ratio of the ionizing flux to the gas density at that location. A temperature-density relation as the one shown in Fig. 5 thus ignores the local variations of the diffuse-field intensity and shape. The large scatter shown in Fig. 5 is therefore a shortcoming of this method, but has the advantage of avoiding the large computational overheads of a full diffuse-field calculation. We stress, however, that the effect of these errors on the dynamics is not large. Again, the error introduced by assuming the particle to be in the cold phase due to the lack of diffuse radiation is much larger than the spread in this relation.

4.3 Step (iii): implement temperature corrections

Once a simple description of the temperature distribution in the shadow region is available from step (ii), this can be implemented as a correction to the SPH temperatures and thus pressure. In the case of the current VINE implementation, this simply requires that at every dynamical time-step, all particles that fulfil the criteria defined in steps (i) and (ii) be identified and their temperature reassigned according to the parametrized curve obtained in step (ii). To avoid unphysical heating far beyond the ionization front, we impose an additional constraint. A particle only gets heated if the total ionized mass inside the current slab perpendicular to the infalling radiation is smaller than the diffusively heated mass inside this slab. Note that this constraint implies that in the last diffusively heated slab, all radiation emitted by recombinations is only absorbed in the adjacent cold structures and not in the hot surrounding gas. This therefore represents the case for maximum efficiency for the diffuse radiation, but, as demonstrated in Section 5.1, we find that no significant overheating of the shadows is introduced by our procedure.

We note that this approach in principle allows for environmental variables, such as the hardness of the stellar field and the metallicity and dust content of the gas to be accounted for in the SPH calculation, since their effect on the temperature distribution is folded in the parametrization obtained with MOCASSIN. In most cases, however, environmental effects on the temperature may be smaller than the scatter showed by the temperature points in Fig. 5.

In the simple implementation of the method presented here, we apply a density cut to the particles to be heated by the diffuse field, which allows us to use a rough but fast criterion for the identification of the diffuse-field-dominated particles without overestimating the effects of the diffuse field. As shown in Fig. 5, the temperature only varies by approximately 50 per cent for number densities lower than $100 \text{ cm}^{-3}$, meaning that the qualitative behaviour of the system would not change significantly if an average value for the temperature were to be used in place of equation (3). The application of equation (3), however, does not add a significant computational overhead, and it is therefore preferred here in view of future calculations where we aim at refining the method to allow the application of a temperature correction to the whole density range, where the temperature variation is larger and the application of a single temperature value would yield larger errors.
5 DIFFUSE-FIELD EFFECTS ON HYDRODYNAMICS

We have compared the results of the original iVINE run with those obtained after implementing the diffuse-field strategy outlined in the previous section. We will refer to the diffuse-field implementation of iVINE as DiVINE (Diffuse-field iVINE).

5.1 Temperature structure in the shadows

As an a posteriori check of the diffuse-field implementation in DiVINE, we compare the gas temperatures at individual slices in the simulation at times 250 and 500 kyr in Figs 6 and 7, respectively. The top right-hand panel and bottom left-hand and right-hand panels show the gas temperatures calculated using iVINE, DiVINE and MOCASSIN, respectively, for the density field shown in the top left-hand panels. We find that, while there are still some obvious differences between the DiVINE and MOCASSIN results, the improvement over the original iVINE runs is certainly encouraging, particularly when considering the minimal computational overhead introduced by this procedure. We also note that the diffuse-field-heated mass in DiVINE and MOCASSIN are very similar.

Some notable differences that can be seen in Figs 6 and 7 include a hot region predicted by DiVINE in Fig. 6 approximately at \((x, y) = (2.2, 0.7)\) pc which is not present in MOCASSIN and cooler regions at large \(x\) predicted by MOCASSIN in Fig. 7. These are both examples in which material in the true shadow has been erroneously been heated by our diffuse-field algorithm in DiVINE. This only represents a small quantity of gas and has no significant effect on the dynamical evolution of the system.

5.2 Clumps, pillars and horse heads

Fig. 1 shows the evolution of the surface density distribution for the standard iVINE run (upper panels) and the DiVINE run (lower panels). The figure suggests that the heating of low-density gas by the diffuse field in the shadow regions results in a clumpier medium at late times. Comparison of volume density slices, like those shown at \(t = 500\) kyr in Fig. 8, further highlight that a clear effect of the inclusion of the diffuse field is that the pillars are eroded from the back, promoting the detachment of clumps. This effect is less visible in integrated surface density maps as those shown in Fig. 1.

The detailed comparison of the main structure obtained with DiVINE to the one obtained in G09b is given in Table 1. The regions compared are marked by the white boundaries drawn on the left-hand panels of Fig. 1. It is interesting to see that the total mass is not strongly affected. However, the DiVINE structure is denser and spatially thinner. The higher density leads to a slower motion away from the ionizing source. By tracing the particles backwards in time, we are able to determine that 75 per cent of the material of the pillar in G09b ends up inside the pillar in DiVINE as well. Another effect of the higher density is enhanced triggered star formation. At \(t = 500\) kyr, the star formation is still identical to G09b. The first star forms in the tip of the secondary pillar, at the same location and with similar properties as before. After that, the star formation is different. A second star forms in DiVINE at the tip...
Figure 7. Density and temperature maps for the $z = 25$ slice of the G09b turbulent ISM simulation at $t = 500$ kyr. Top left-hand panel: gas density map. Top right-hand panel: electron temperature, $T_e$, as calculated by iVINE. Bottom left-hand panel: electron temperature, $T_e$, as calculated by DiVINE. Bottom right-hand panel: electron temperature, $T_e$, as calculated by MOCASSIN with nebular abundances.

Figure 8. Volume density slices at $t = 500$ kyr for the iVINE (left-hand panel) and DiVINE (right-hand panel) runs.

of the primary pillar after $t \approx 525$ kyr, while it forms much later in the G09b simulation (at $t \approx 735$ kyr).

Altogether, the overall evolution is similar and the formation of structures is still governed by the initial turbulence, especially in high-density regions, which are only weakly affected by diffuse radiation. However, small-scale dynamics and especially the triggered star formation change due to the inclusion of diffuse radiation.

We have also considered the observational appearance of such clumpy structures in typical narrow-band filters by computing the Hα and [O iii]λλ5007,4659 line emission and producing a
false-colour image along a line of sight parallel to the z-axis. We used the interstellar extinction curve of Weingartner & Draine (2001) for a Milky Way size distribution for $R_V = 3.1$, with $C/H = b_c = 60$ ppm in lognormal size distributions, but renormalized by a factor of 0.93. This grain model is considered to be appropriate for the typical diffuse H I cloud in the Milky Way. The result is shown in Fig. 9, which shows ‘pillar-like’ as well as ‘horse-head-like’ structures very much resembling the famous Hubble Space Telescope images. Hence, even though the structures are mostly detached from the parent cloud, the appearance is still that of coherent pillars.

5.3 PI-driven turbulence

G09b found that turbulence on small scales could be sustained by the ionizing radiation. We have revisited this question using the results obtained from DiVINE, and we confirm the general conclusion that turbulence is driven by ionizing radiation. A comparison of the iVINE and DiVINE turbulence spectra can be seen in Fig. 10, where we plot the specific energy as a function of wavenumber (large wavenumbers = small spatial scale) for the original control run with no ionizing radiation presented by G09b (dotted lines), G09b’s standard iVINE run (dashed lines) and the DiVINE run presented in this work (solid lines). The efficiency of the driving is slightly reduced in the DiVINE calculations. We ascribe this effect to the higher compression of the cold gas due to the existence of the diffuse phase. The cold gas therefore experiences more shocks initially and is constrained more tightly, leading to lower turbulent motions.

6 CONCLUSIONS

We have presented a detailed comparison of the ionization and temperature structure for a turbulent ISM simulation performed with the SPH + ionization code iVINE (Gritschneder et al. 2009a, 2010; G09b) against the solution obtained with the PI code MOCASSIN for snapshots of the density distribution. iVINE treats hydrodynamics, gravitational forces and ionization simultaneously. The ionization is calculated by making use of the ‘OTS’ approximation. The MOCASSIN code (Ercolano et al. 2003, 2005, 2008a) is fully three dimensional and includes an exact treatment for the frequency-resolved transfer of both the stellar (direct) and diffuse radiation fields. MOCASSIN includes all the microphysical processes that dominate the thermal and ionization balance of the ionized gas, providing realistic temperature and ionization distributions.

Our tests show that iVINE and MOCASSIN agree very well on the global properties of the region (i.e. total ionized mass fraction and location of the main ionization front), but we note discrepancies in the temperature structure, particularly in the shadow regions. These tend to be cold and neutral in the iVINE plane-parallel stellar-field-only prescription, while MOCASSIN obtains a range of ionization levels and temperatures that can be very crudely described as a function of density.

We have developed a computationally inexpensive strategy to include the thermal effects of the diffuse field, as well as accounting for environmental variables, such as gas metallicity and stellar spectra hardness. The method relies on the identification of the shadow region via simple criteria and application of a temperature parametrization that was obtained a priori using MOCASSIN.

| Simulation | $M$ (M$_\odot$) | $\rho_0$ ($m_p$ cm$^{-3}$) | $\Sigma$ (g cm$^{-2}$) | $\sigma$ (km s$^{-1}$) | $\bar{v}_x$ (km s$^{-1}$) |
|------------|-----------------|-----------------------------|------------------------|-------------------------|--------------------------|
| G09b       | 12.6            | $4.56 \times 10^4$         | $1.52 \times 10^{-3}$  | $1.1 \pm 0.7$          | $4.8 \pm 0.9$            |
| DiVINE     | 12.0            | $6.33 \times 10^4$         | $1.89 \times 10^{-3}$  | $0.9 \pm 0.5$          | $4.2 \pm 0.8$            |

Table 1. Comparison of DiVINE and iVINE at $t = 500$ kyr. Listed are the mass, mean density, mean surface density, velocity dispersion and the $x$-velocity away from the source of the most prominent structure. As the structure is not homogeneous, we also include the standard deviation across the structure for both velocities.

Figure 9. False colour composite image of the DiVINE simulation at $t = 500$ kyr. Red = H$_\alpha$, blue = [OIII]$\lambda\lambda 5007,4959$ and green = combination.

Figure 10. Specific energy as a function of wavenumber. Dotted lines: iVINE run with no ionization. Solid lines: iVINE run. Dashed lines: DiVINE run...
method can be readily extended to other hydrodynamical codes (both SPH and grid based).

We evaluate the effects of diffuse fields by comparing runs with the standard iVINE and the diffuse-field implementation DVINE. In agreement with previous studies (Raga et al. 2009), we find that the overall qualitative behaviour of the system (i.e. the formation of what appear to be pillar-like structures) is similar in the two runs. Nevertheless, our models demonstrate that the diffuse field has important quantitative effects on the hydrodynamical evolution of the irradiated ISM. In particular, we note that DVINE predicts denser and less coherent structures which are much less attached to the parental cloud. This is due to the higher compression of the cold structures by the diffusively heated material inside the pillars’ trunks. Triggered star formation is promoted by this effect to a much earlier time. The compression also affects the turbulence spectrum of the system. We confirm the driving of turbulence by the ionizing radiation, but with a slightly reduced efficiency compared to previous calculations with iVINE using the OTS approximation.

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