The effects of spatially distributed ionisation sources on the
temperature structure of H II regions

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ABSTRACT

Spatially resolved studies of star forming regions show that the assumption of spherical geometry is not realistic in most cases, with a major complication posed by the gas being ionised by multiple non-centrally located stars or star clusters. Geometrical effects including the spatial configuration of ionising sources affect the temperature and ionisation structure of these regions. We try to isolate the effects of multiple non-centrally located stars, via the construction of 3D photoionisation models using the 3D Monte Carlo photoionisation code MOCASSIN with very simple gas density distributions, but various spatial configurations for the ionisation sources. Our first aim is to study the resulting temperature structure of the gas and investigate the behaviour of temperature fluctuations within the ionised region. We show that geometry affects the temperature structures in our models differently according to metallicity. For the geometries and stellar populations considered in our study, at intermediate and high metallicities, models with ionising sources distributed in the full volume, whose Strömgren spheres rarely overlap, show smaller temperature fluctuation than their central ionisation counterparts, with fully overlapping concentric Strömgren spheres. The reverse is true at low metallicities. Finally the true temperature fluctuations due to the stellar distribution (as opposed to the large-scale temperature gradients due to other gas properties) are small in all cases and not a significant cause of error in metallicity studies.

Emission line spectra from H II regions are often used to study the metallicity of star-forming regions, as well as providing a constraint for temperatures and luminosities of the ionising sources. Empirical metallicity diagnostics must often be calibrated with the aid of photoionisation models. However, most studies so far have been carried out by assuming spherical or plane-parallel geometries, with major limitations on allowed gas and dust density distributions and with the spatial distribution of multiple, non-centrally located ionising sources not being accounted for. We compare integrated emission line spectra from our models and quantify any systematic errors caused by the simplifying assumption of a single, central location for all ionising sources. We find that the dependence of the metallicity indicators on the ionisation parameter causes a clear bias, due to the fact that models with a fully distributed configuration of stars always display lower ionisation parameters than their fully concentrated counterparts. The errors found imply that the geometrical distribution of ionisation sources may partly account for the large scatter in metallicities derived using model-calibrated empirical methods.

Key words: (ISM): H II regions; galaxies: abundances; radiative transfer

1 INTRODUCTION

The ability to measure accurate chemical abundances in H II regions in our own and other galaxies is vital for our understanding of
their chemical evolution. Emission lines emitted by the nebular gas photoionised by massive stars provide us with powerful metallicity indicators for near and intermediate redshift galaxies. The major complication is posed by the critical task of determining the physical parameters of the nebula, in particular the electron temperature, $T_e$. Failure to achieve realistic estimates may lead to gross errors in the final abundance determination. Temperature fluctuations within the nebula may be an important cause of error. Collisionally excited lines (CELs), which are routinely used in abundance studies, are naturally weighted towards hotter regions and may therefore lead to underestimating of the real abundances. Recombination lines (RLs) are less affected by errors in temperature determinations, and should in theory yield more accurate results. One of the outstanding problems in nebular astrophysics is the discrepancy between abundances and electron temperature estimates obtained from CELs or RLs in Planetary Nebulae (PNe) (e.g. Rubin et al. 2002; Wesson, Liu & Barlow 2005; Ercolano et al. 2005; Liu et al. 2006; Peimbert & Peimbert 2006 and references therein), galactic and Magellanic H II regions (e.g. Peimbert, Peimbert & Ruiz 2000; Peimbert 2003; Tsamis et al. 2003; Esteban et al. 2004; García-Rojas et al. 2005, 2006) and extragalactic H II regions (e.g. Peimbert & Peimbert 2003; Peimbert & Ruiz 2005). The cause of this discrepancy is still uncertain; temperature fluctuations and chemical inhomogeneities in the gas have both been advocated to explain the discrepancy. Photoionisation models including chemical inhomogeneities have been successful in matching the observed CEL and RL spectra of some PNe (e.g. Ercolano et al. 2003b) and H II regions (Tsamis & Péquignot 2005). However the discrepancy between the abundances derived from recombination lines (RL) and those derived from CELs has been also been attributed to temperature fluctuations not caused by abundance inhomogeneities (e.g. García-Rojas et al. 2004). The $I^2$ parameter (Peimbert, 1967; Peimbert & Costero 1969; Peimbert 1971), introduced in order to quantify such fluctuations, can be derived empirically by the comparison of temperatures obtained from the depth of the Balmer Jump to those obtained from CELs. Although the situation for H II regions is notoriously less worrying than for PNe, the problem still remains that empirically determined $I^2$ values are larger than those indicated by chemically homogeneous photoionisation models, indicating that the causes of the proposed temperature fluctuations are still not understood.

Aside from temperature fluctuations the task of obtaining reliable abundance estimates from CEL spectra of H II regions is further complicated by the fact that often the complete set of emission lines needed for a direct measurement of the electron temperatures is not available for all sources; the 4363 Å line of [O III] and the 5755 Å line of [N II] are weak and therefore not detected if the spectra do not have good signal-to-noise or if the metallicities are high, implying low electron temperatures. A large effort has been made to provide metallicity and temperature indicators based on various combinations of strong lines (e.g. Pagel et al. 1979; Allin et al. 1979; Mc Gaugh 1991; Storchi-Bergmann et al. 1994; Vilchez & Esteban 1996; Van Zee et al. 1998; Pilyugin 2001a; Pettini & Pagel 2004; Pérez-Montero & Díaz 2005). Hägele et al. (2006) have recently proposed a new methodology for the production and calibration of empirical relations between the different line temperatures based on observational data alone. However the data sets available are still too limited to provide usable indicators. Currently, calibrations of metallicity indicators and ionic temperature relations are generally not based on observational data alone, but make use of grids of photoionisation models, run for a range of metallicities and ionisation parameters (e.g. McGaugh 1991, Charlot & Longhetti 2001, Kewley & Dopita 2002). Given the vast parameter space generally under investigation, most studies so far have been carried out with spherically symmetric or plane parallel geometries, with major limitations on the allowed density distribution and with the spatial distribution of the ionising sources not being investigated. Nearby H II regions, however, show complex structures in the distribution of gas and stars, which are often intermixed.

In this paper we carry out a theoretical investigation of the importance of the effects due to the spatial distribution of the ionising sources via the construction of a number of 3D photoionisation models, using the MOCASSIN code (Ercolano et al. 2003a, 2005) for simple gas density distributions and three spatial configurations for the ionisation sources.

Our modelling strategy is described in Section 2. Temperature fluctuations are estimated for our models by computing theoretical $I^2$ and $T_e$ values (Peimbert, 1967) for each of our models and the results are given and discussed in Section 3. In this Section we also compare integrated emission line spectra from such configurations to search for systematic errors which may be caused by the simplifying assumption of a single, central location for all ionising sources. We also test the robustness of a number of commonly used ionic temperature relations. A summary of our main results is presented in Section 4.
Table 2. Model grid legend. H number density, \( N_H = 100 \) \( \text{cm}^{-3} \) for all models. Figures in this paper rely on colour, please refer to on-line version. For black and white copies black is black, blue is dark-gray, red is medium gray and green is light gray.

| model     | star distrib. | geometry | Z/Z⊙ | symbol          | model     | star distrib. | geometry | Z/Z⊙ | symbol          |
|-----------|----------------|-----------|------|-----------------|-----------|----------------|-----------|------|-----------------|
| CSp2.0    | central        | sphere    | 2.0  | small magenta circle | CSh0.4    | central        | shell     | 0.4  | small red square |
| HSp2.0    | half distrib   | sphere    | 2.0  | medium magenta circle | HSh0.4    | half distrib   | shell     | 0.4  | medium red square |
| FSp2.0    | fully distrib  | sphere    | 2.0  | large magenta circle | FSh0.4    | fully distrib  | shell     | 0.4  | large red square |
| CSh2.0    | central        | shell     | 2.0  | small magenta square | CSp0.2    | central        | sphere    | 0.2  | small green circle |
| HSh2.0    | half distrib   | shell     | 2.0  | medium magenta square | HSp0.2    | half distrib   | sphere    | 0.2  | medium green circle |
| FSh2.0    | fully distrib  | shell     | 2.0  | large magenta square | FSp0.2    | fully distrib  | sphere    | 0.2  | large green circle |
| CSp1.0    | central        | sphere    | 1.0  | small black circle | CSh0.2    | central        | shell     | 0.2  | small green square |
| HSp1.0    | half distrib   | sphere    | 1.0  | medium black circle | HSh0.2    | half distrib   | shell     | 0.2  | medium green square |
| FSp1.0    | fully distrib  | sphere    | 1.0  | large black circle | FSh0.2    | fully distrib  | shell     | 0.2  | large green square |
| CSh1.0    | central        | shell     | 1.0  | small black square | CSp0.05   | central        | sphere    | 0.05 | small green circle |
| HSh1.0    | half distrib   | shell     | 1.0  | medium black square | HSp0.05   | half distrib   | sphere    | 0.05 | medium green circle |
| FSh1.0    | fully distrib  | shell     | 1.0  | large black square | FSp0.05   | fully distrib  | sphere    | 0.05 | large green circle |
| CSp0.4    | central        | sphere    | 0.4  | small red circle  | CSh0.05   | central        | shell     | 0.05 | small green square |
| HSp0.4    | half distrib   | sphere    | 0.4  | medium red circle  | HSh0.05   | half distrib   | shell     | 0.05 | medium green square |
| FSp0.4    | fully distrib  | sphere    | 0.4  | large red circle  | FSh0.05   | fully distrib  | shell     | 0.05 | large green square |

2 MODELLING STRATEGY

The aim of the current investigation is to uncover possible systematic differences on the temperature structure and emission line spectra of nebulae ionised by a centrally concentrated set of stars or clusters versus those ionised by the same set of sources which are randomly distributed within the half or full volume, whose respective Strömgren spheres do or do not overlap. In particular we want to test which of the stellar configurations considered produces the largest temperature fluctuations and of what magnitude. At this stage we do not attempt to assess the absolute strengths and weaknesses of one metallicity indicator or ion temperature relation over others, a task that may only be carried out by a systematic investigation of the large parameter space. In an attempt to isolate the effects of the stellar distribution from those due to the gas density distribution, we consider two extremely simple geometries - a homogeneous spherical volume and a homogeneous spherical shell, both of constant hydrogen number density, \( N_H = 100 \) \( \text{cm}^{-3} \). The shell models have inner radii of \( 2.8 \times 10^{18} \) cm and Strömgren radii (corresponding to the case when all stars are located at the centre) as listed in Table 2. The total number of ionising photons is constant for all models and is \( Q_{\text{HI}} = 3.80 \times 10^{50} \text{ sec}^{-1} \).

For each density distribution we are interested in a comparison between the centrally concentrated and the half and fully distributed source cases. In the remainder of this paper we will refer to models ionised by a central concentration of stars as models C, those ionised by the same set of stars distributed in the half and full volumes will be referred to as models H and F, respectively. Case C is equivalent to models ionised by a single central source with a total bolometric luminosity equal to the sum of the bolometric luminosities of the individual sources (as given in Table 2) and a spectral shape given by the superposition of the spectra of all sources. These models could also be performed using a 1D code, with a spherically symmetric gas density distribution. Similarly a 1D code could also be employed for case F models where the Strömgren spheres do not generally overlap the left panel of Figure 1 shows a 3D representation of the Strömgren sphere distribution for case F, plotted as iso-surfaces where the ionisation fraction of hydrogen is 0.95. The adjacent panel shows a projected map of the ionic abundance regions partially overlap; the determination of the radiation field in the overlap region is not possible without the application of a 3D code. As we are interested in a comparison of the three cases (C, H and F), self-consistency is crucial and for this reason we have run all models with the same 3D code, MOCASSIN.

Our models include five metallicities (\( Z/Z⊙ = 0.05, 0.2, 0.4, 1.0, 2.0 \)) and, the "solar" abundance set uses the values from Grevesse & Sauval (1998) with the exception of C, N, O abundances which are taken from Allende Prieto et al. 2002, Holweger 2001 and Allende Prieto et al. 2001, respectively. These were scaled to lower and higher metallicities for the 37 M⊙ and a 56 M⊙ population, with half of the total ionising photon output \( [s^{-1}] \) being emitted by each population. These two stellar masses were chosen as they have very different \( Q_{\text{He},0}/Q_{\text{H},0} \) ratios, where \( Q_{\text{HI}} \) is the total output \( [s^{-1}] \) of H-ionising photons (energy > 1 ryd) and \( Q_{\text{He},0} \) is the total output \( [s^{-1}] \) of He-ionising photons (energy > 1.8 ryd), and are likely to produce the largest effects on the temperature structure and sharpness of the ionisation front. The ionising spectra for single-mass stars were computed with the STARBURST99 spectral synthesis code Leitherer et al. (1999) with the up-to-date non-LTE stellar atmospheres implemented by Smill, Norris & Crowther (2002), using single isochrones for the appropriate stellar masses. The models were calculated at metallicities consistent with the nebular gas and were obtained for an instantaneous burst, at an age of 1 Myr. At solar metallicities for the 37 M⊙ stars, the stellar atmosphere models possible that a small fraction of them may actually have partially overlapping Strömgren spheres.

1 Due to the stochastic nature of the ionisation source distribution, it is possible that a small fraction of them may actually have partially overlapping Strömgren spheres.
emit 32.3% of luminosity in the H-ionising continuum and 7.7% in the He-ionising continuum, while for the 56 $M_\odot$ stars these percentages are 47.9% and 13.7%, respectively. The exact percentages vary with stellar metallicity, nevertheless the values above are given as a guide to appreciate the different spectral hardness of the two populations.

Some other defining parameters of our models, together with their nomenclature and associated symbols are given in Table 2.

2.1 The 3D photoionisation code: MOCASSIN

The 3D photoionisation code MOCASSIN (Ercolano et al. 2003a, 2005) uses a Monte Carlo approach to the radiation transport problem and it is therefore completely independent of geometry and density distribution. Both the stellar and diffuse components of the radiation field are treated self-consistently, without the need of approximations. Multiple ionisation sources can be located at arbitrary positions in the simulation grid with the only limit being imposed by computing resources. The atomic data used is frequently updated and include sets of energy levels, collision strengths and transition probabilities from Version 5 of the Chianti database (Landi et al., 2005) and the improved H i, He i and He ii free-bound continuous emission data recently published by Ercolano & Storey (2006). A public version of the FORTRAN 90 code, which is fully parallelised using the Message Passing Interface (MPI) libraries, can be obtained from B. Ercolano. Version 2.02.38 was used for the models presented in this work. We simulate one quadrant of each model, using the technique described and tested by Ercolano et al. (2003b), whereby the positive x-y, y-z and x-z planes intersecting the z-, x- and y- axes respectively at zero, act as mirrors, reflecting the incoming photons back into the simulated cube. The full volume is finally described by $10^6$ cells for the spherical models ionised by 240 sources. The number of energy packets used varies during the course of our simulations, but typically 1-10 million packets are sufficient for our grids to reach convergence within 10-20 iterations. We experimented with higher resolution grids and a larger number of energy packets and found our results to be virtually unaffected.

2.2 Validation of our models

As stated above, the aim of this paper is not to provide new calibrations to abundance diagnostic ratios nor to assess their absolute accuracy. It is therefore not in our intention to create models that may introduce errors in the empirical calculations of abundances, examined. The robustness of commonly used abundance diagnostics and ionic temperature relations are also tested against possible errors introduced by geometrical effects.

3 RESULTS

The temperature structure and emission line spectra obtained by our models are analysed here in detail. Temperature fluctuations, which may introduce errors in the empirical calculations of abundances, are examined. The robustness of commonly used abundance diagnostics and ionic temperature relations are also tested against possible errors introduced by geometrical effects.

3.1 Temperature structure

The volume integrated electron temperatures weighted by a number of commonly observed ionic species are plotted in Figure 2 for metallicities of $Z/Z_\odot = 0.05, 0.2, 0.4, 1$ and $2$. The values were obtained according to

$$T_e(X^{+i}) = \frac{\int N_e N(X^{+i})T_e\, dV}{\int N_e N(X^{+i})\, dV}$$

The models are represented by circles and squares of various colours and sizes as described in Table 2.

At a first glance some trends are apparent. At solar and high metallicities (i.e. $Z/Z_\odot \geq 1$) the electron temperatures in ‘high’ ionic species zones (e.g. O III, S III, Ar III and N III) are higher for models in cases H and F. The opposite is true for electron temperatures in ‘low’ ionic species zones, such as O II and N II. This implies a shallower temperature gradient for case F and H when compared to case C, since at these metallicities the highest nebular temperatures are reached in the low ionisation zones which are not affected by the very efficient cooling provided by the IR fine-structure lines of [O III] as in the high ionisation zones, where, in fact, the lowest temperatures are reached. The $Z/Z_\odot = 0.05$ and 0.2 models do not follow the same trend; here there is a monotonic shift of temperatures, whereby C models are hotter than the H and F models, regardless of ionic species zone. At intermediate metallicities ($Z/Z_\odot = 0.4$) we are in a transition case from the two separate behaviours described above. At low metallicities, the cooling is dominated by collisional excitation of H Ly$\alpha$, which increases as one gets closer to the ionisation front, where the proportion of residual neutral hydrogen increases. This results in a outward decreasing temperature, contrary to the high metallicity cases.

Differences in the temperature structure of cases F and C can be understood as follows: at each point in the nebula the electron temperature is primarily determined by the average energy of the photons absorbed by H and He and by the cooling efficiency of the
ions. The latter is naturally less important at lower metallicities. However, for the intermediate to high metallicity cases, it is differences in the distribution of the cooling ions rather than differences in the heating rates which explains the difference in temperature structure between case C and case H for higher and intermediate metallicities.

3.2 Temperature Fluctuations

We have calculated for the main ionic species in our models the formal values of the mean ionic temperatures, $T_0$, and of the temperature fluctuations, $t^2$, according to the formalism of Peimbert (1967). Note that in the case of concentric sources, $t^2$ measures changes in radial gradients of the temperature rather than “temperature fluctuations” while in the cases of distributed sources it really represent a temperature fluctuation. For brevity we only list the values for H$^+$, O$^+$ and O$^{2+}$ in Table 3.1. The errors quoted in the table are representative of the accuracy achieved by our models. They contain contributions from the variance intrinsic to our Monte Carlo approach and the error introduced by using a finite grid to describe the ionised region. The errors were estimated by considering that for a fully spherically symmetric case, such as one with homogeneous gas density distribution and a central location for all ionising sources, the $t^2$ in an infinitely narrow spherical shell centred on the source of the ionising photons should be zero. We note that our errors increase with increasing metallicities, this is due to the larger temperature gradients occurring at higher metallicities causing the error contribution due to the finite grid description to increase. Clearly all errors could be reduced by increasing the number of energy packets and grid cells used in the simulations. However we note that our errors are always at least one order of magnitude smaller than the $t^2$ values and therefore do not affect our conclusions. Given the large number of 3D models run for this work (which vastly exceeds those finally presented here), we feel that a good balance between accuracy and computational expense was achieved.

The value of $t^2(O^+)$ is very hard to derive empirically. We know however of three H II regions where this measurement has been made: the Orion nebula (Esteban et al. 2004), M20 (García-Rojas et al., 2006) and M8 (García-Rojas et al. 2007). In those cases where $t^2(O^+)$ cannot be derived empirically, it is generally assumed that $t^2(O^+) = t^2(O^{2+})$; it is clear from the values listed in our table that this assumption is very often not verified and care should be taken to account for this in the error estimation from such studies. For our $Z/Z_\odot = 2$ models, $t^2(O^{2+})$ is always a factor of 2 or more higher than $t^2(O^+)$, while for lower metallicities...
$t^2(O^{2+})$ becomes lower than $t^2(O^+)$. Finally, we note that the formal $t^2$ values may diverge from the empirical ones (e.g. Kingdon & Ferland, 1995; Zhang, Ercolano & Liu, 2007), that are generally based on the comparison of the electron temperature derived from the depth of the Balmer jump and the $[O III]$ temperature, the values listed in Table 3.1 are, nevertheless, sufficient to identify the effects of the stellar distribution on temperature fluctuations in the nebular gas.

In Figure 5, we plot the $t^2$ values for $H^+$ and $O^{2+}$ (dashed and solid lines, respectively) against metallicity for the spherical and shell models. Cases C, H and F are represented by black, red and green lines and symbols respectively. Unsurprisingly, the temperature fluctuations, which in this case are a direct consequence of large-scale temperature gradients, are larger for the high metallicity models. A full discussion of this effect and of the causes of the large scale temperature fluctuations in metal rich nebulae is given by Stasińska (1980) and Kingdon & Ferland (1995). What had not been noticed before, however, is that at very low metallicities, the $t^2$ values for $H^+$ and $O^+$ rise again; this is due to the large temperature gradient already shown in Figure 4. However, $t^2(O^{2+})$ remains tiny, so that the overall effect on abundance determinations is expected to be small.

With regards to a comparison of the $t^2$ values obtained with the three different spatial distributions of sources (cases C, H and F), we first of all notice that for intermediate to high metallicities ($Z/Z_\odot \geq 0.4$), case F models show a more isothermal gas (smaller $t^2$) than case H or C models. This is due to the fact that the contributions to the $t^2$ due to the true temperature fluctuations created by the two different stellar populations in case F (and in a smaller degree in case H) are completely washed out by the large-scale temperature gradients caused by the metals’ cooling. This effect vastly dominates at these metallicities, resulting in larger values of $t^2$ being obtained by case C models, which, as discussed in the previous section (see Figure 4), have steeper temperature gradients than their cases H and F counterparts.

The above is further confirmed by the fact for very low metallicities ($Z/Z_\odot \leq 0.2$), case F models (green lines) show larger fluctuations than case C and H models. This is because at these low metallicities, case C, H and F all show similar large-scale temperature gradients (see Figure 4); the values of $t^2$ are thus larger for case F models where true temperature fluctuations are at play. However, once again we point out that no large effects are expected on abundance determinations due to the fact that $t^2(O^{2+})$ is small in all cases.

**Figure 3.** H II region ionisation sequence parametrised in terms of oxygen and sulphur. The grey dots indicate the position of giant H II regions in spiral galaxies taken from Garnett & Kennicutt (1994), Garnett et al. (1997), van Zee et al. (1998), Bresolin et al. (1999, 2004, 2005), Kennicutt et al. (2003), spanning metallicities from $12 + \log(O/H) \sim 8$ to $\sim 8.8$. The top right panel also includes a few points from metal-poor emission line galaxies from Izotov et al. (2006), which extend to $12 + \log(O/H) \sim 7.2$; it was not possible to use this data for the other three panels, due to the lack of simultaneous detection of all the lines needed. The symbols and colors correspond to our models as defined in Table 2. Please refer to the on-line version of this paper for colour figures.
3.3 Ionic temperature relations

We have shown that the temperature structure of models with centrally concentrated ionising sources, case C, may vary compared to those of similar models where the sources are distributed within the half volume (case H), which have partially overlapping Strömgren spheres, and to those with sources distributed within the full volume (case F), which have fully independent Strömgren spheres. Case C to case F variations in the temperature structure of the models may have implications for a number of ionic temperature relations. These scaling laws are often employed in abundance studies when observational data for a given ionic zone is missing. Some of the most popular relations we found in the literature include \( T_{\text{e}}(\text{S}^\text{III}) \) vs \( T_{\text{e}}(\text{Ar}^\text{III}) \), \( T_{\text{e}}(\text{O}^\text{III}) \) vs \( T_{\text{e}}(\text{Ar}^\text{III}) \), \( T_{\text{e}}(\text{O}^\text{II}) \) vs \( T_{\text{e}}(\text{N}^\text{II}) \). These ratios are expected to be around unity and we found them to be very little affected by the shifts in temperatures due to the spatial distri-
Figure 5. Mean ionic temperatures and temperature fluctuations as a function of gas metallicity for the homogeneous sphere and shell models. $T_2(O^{2+})$ and $T_2(H^+)$ are represented by solid and dashed lines, respectively. The lines are colour coded such that black, red and green are for cases C, H and F, respectively. Please refer to the on-line version of this paper for colour figures.

Figure 6. $T_2(O\ II)$ versus $T_2(O\ III)$ for $Z/Z_\odot=1.0$ and $2.0$ left and $Z/Z_\odot=0.05, 0.2$ and $0.4$ right models for cases C, H and F. The straight black solid line is the scaling law of Garnett (1992) and the blue dotted and red dashed curves are the relations given in Eqn 14 of Izotov et al. (2006) for $12 + \log(O/H) = 8.2$ (red), 7.6 (blue dotted, thick) and 7.2 (blue dotted, thin). The symbols representing our models are described in Table 2. Please refer to the on-line version of this paper for colour figures.
involved are both 'high' (O II) and 'low' (O III) population of stars. This is not surprising, given that the ionicspecies remain virtually unaffected.

Each case may shift to higher or lower values, the resulting ratios therefore plotted in blue in the right panel of our Figure 6, with the thinner and thicker curves indicating the 7.2 and 7.6 metallicity bin, respectively. Our Z/Z⊙金属licity bin, which, nevertheless is represented by the model, is much more affected by the fact that low and high ionic temperatures shift in opposite directions for intermediate (red points; Z/Z⊙ = 0.4) and high metallicities (magenta and black points; Z/Z⊙ = 2 and 1). This

| Model | T0(H+) | t²(H+) | T0(OIII) | t²(OIII) | T0(OII) | t²(OII) |
|-------|--------|--------|---------|---------|--------|--------|
| CSphH0.05 | 18240 | 0.0178 | 13350 | 0.041 | 18500 | 0.007 |
| HSphH0.05 | 17690 | 0.0228 | 12830 | 0.046 | 18500 | 0.007 |
| FSphH0.05 | 14850 | 0.0511 | 11720 | 0.035 | 17180 | 0.009 |
| ± 0.0006 | ± 0.003 | ± 0.004 | ± 0.004 | ± 0.004 | ± 0.004 | ± 0.004 |
| CSphH0.2 | 13140 | 0.0034 | 12060 | 0.0145 | 13430 | 0.0010 |
| HSphH0.2 | 13230 | 0.0036 | 11810 | 0.0156 | 13430 | 0.0005 |
| FSphH0.2 | 12100 | 0.0112 | 11160 | 0.0141 | 12860 | 0.0010 |
| ± 0.0001 | ± 0.0004 | ± 0.0004 | ± 0.0004 | ± 0.0004 | ± 0.0004 | ± 0.0004 |
| CSphH0.4 | 9850 | 0.0063 | 10620 | 0.0069 | 9790 | 0.0053 |
| HSphH0.4 | 9860 | 0.0038 | 10500 | 0.0060 | 9790 | 0.0029 |
| FSphH0.4 | 9710 | 0.0036 | 9910 | 0.0047 | 9600 | 0.0024 |
| ± 0.0005 | ± 0.0007 | ± 0.0007 | ± 0.0007 | ± 0.0007 | ± 0.0007 | ± 0.0007 |
| CSphH1.0 | 6690 | 0.024 | 8130 | 0.020 | 6380 | 0.012 |
| HSphH1.0 | 6670 | 0.021 | 8110 | 0.020 | 6380 | 0.009 |
| FSphH1.0 | 7320 | 0.018 | 7990 | 0.012 | 6710 | 0.009 |
| ± 0.0006 | ± 0.002 | ± 0.002 | ± 0.002 | ± 0.002 | ± 0.002 | ± 0.002 |
| CSphH2.0 | 5000 | 0.156 | 6110 | 0.043 | 2910 | 0.130 |
| HSphH2.0 | 4880 | 0.152 | 5980 | 0.050 | 2919 | 0.096 |
| FSphH2.0 | 5360 | 0.075 | 5890 | 0.036 | 3700 | 0.084 |
| ± 0.0005 | ± 0.003 | ± 0.003 | ± 0.003 | ± 0.003 | ± 0.003 | ± 0.003 |
| CSphH0.05 | 17510 | 0.0129 | 13770 | 0.0437 | 18110 | 0.0041 |
| HSphH0.05 | 17520 | 0.0166 | 13440 | 0.0438 | 18110 | 0.0057 |
| FSphH0.05 | 15200 | 0.0369 | 12410 | 0.0348 | 16840 | 0.0098 |
| ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 |
| CSphH0.2 | 12940 | 0.0033 | 12390 | 0.0113 | 13210 | 0.0017 |
| HSphH0.2 | 13080 | 0.0029 | 12250 | 0.0124 | 13210 | 0.0010 |
| FSphH0.2 | 12280 | 0.0082 | 11520 | 0.0121 | 12810 | 0.0015 |
| ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 | ± 0.0002 |
| CSphH0.4 | 9780 | 0.0091 | 10570 | 0.0089 | 9710 | 0.0078 |
| HSphH0.4 | 9880 | 0.0084 | 10740 | 0.0081 | 9710 | 0.0068 |
| FSphH0.4 | 9810 | 0.0060 | 10130 | 0.0064 | 9620 | 0.0046 |
| ± 0.0003 | ± 0.0003 | ± 0.0003 | ± 0.0003 | ± 0.0003 | ± 0.0003 | ± 0.0003 |
| CSphH1.0 | 6880 | 0.030 | 7980 | 0.026 | 6460 | 0.017 |
| HSphH1.0 | 6850 | 0.029 | 8010 | 0.026 | 6460 | 0.016 |
| FSphH1.0 | 7280 | 0.021 | 7940 | 0.017 | 6720 | 0.012 |
| ± 0.001 | ± 0.001 | ± 0.001 | ± 0.001 | ± 0.001 | ± 0.001 | ± 0.001 |
| CSphH2.0 | 5450 | 0.086 | 5980 | 0.045 | 3420 | 0.09 |
| HSphH2.0 | 5430 | 0.090 | 6000 | 0.045 | 3420 | 0.09 |
| FSphH2.0 | 5490 | 0.070 | 5950 | 0.037 | 3690 | 0.08 |
| ± 0.006 | ± 0.006 | ± 0.006 | ± 0.006 | ± 0.006 | ± 0.006 | ± 0.006 |
will contribute to the scatter noticed observationally for this relation. For example, Kennicutt, Bresolin & Garnett (2003) presented a study of those H II regions in M 101 for which direct measurements of the nebular auroral lines could be obtained. They found the T_e(O III) vs T_e(S II) relation to be matched closely by their observations, whereas the T_e(O II) and T_e(S II) temperatures turned out to be rather uncorrelated. It is also worth noting at this point that another factor that could contribute to the scatter in the T_e(O III) vs T_e(O II) relation is the dependency of T_e(O II) on the electron density (Pérez-Montero & Díaz 2003). The scatter found by our models is for a given electron density, and therefore it may be even larger for a different sample covering a wider range of densities. The ionising flux distribution is certainly a factor that contributes to weakening the correlation, however, as pointed out by Stasińska (2005), at high metallicities, the temperature derived from the [O ii] line ratio may be strongly in error due to the contribution of recombination from O^{++}.

### 3.4 Abundance diagnostics

We have assessed that the geometrical distribution of stars within an H II region plays a role in the temperature structure of the gas, the magnitude of these effects will clearly be dependent on the total mass of the stars and the concentration level. It is important now to verify the robustness of commonly used metallicity indicators against these temperature shifts. In particular we are interested in identifying systematic trends with stellar distribution rather than absolute errors. Table I lists the empirical oxygen abundances obtained using 6 different indicators. We used the following calibrations for the 6 indicators: (1) O_{23} – Pilyugin (2000, 2001b), (2) O_{3}N_{2} – Stasińska (2006), (3) N_{2} – Pettini & Pagel (2004), (4) S_{23} – Pérez-Montero & Díaz (2005), (5) S_{33}O_{3} – Stasińska (2006), (6) Ar_{3}O_{3} – Stasińska (2006). It is worth reiterating at this point that metallicity indicators should, and generally are, only used for statistical studies as the error on a single region may be very large; the models presented in this work do not attempt to cover the full parameter space occupied by H II regions and therefore do not aim at identifying the most accurate indicator in absolute terms. Here we are mainly interested in studying a possible systematic error in the derived abundances introduced by the 3D stellar distribution. For this reason for each trio of models (C, H and F for a given density distribution and metallicity) we compute \Delta, the largest difference between the oxygen abundance derived from C, H and F.

The results are summarised in Table 4 where the mean values <\Delta> are also listed. For all metallicity indicators apart from O_{23}, there is a clear trend for higher metallicity being derived from models ionised by fully distributed sources, case F, than from case C and H models. The reverse is true for O_{23}, where metallicities derived from case F models are smaller than those derived from case C and H models. The Delta values at a given metallicity vary from one indicator to the next, however they are rarely below \sim 0.1 dex (only for the highest metallicity case), with more representative values around 0.3 dex for the spherical case, but often larger than 0.4 dex. These deviations are slightly smaller for the shell density distributions; this is obvious as even for F cases most of the ionising radiation in these models will be emitted from the central cavity, reducing the differences between C and F cases. We note that in some cases the values given by the case H models are lower than those given by the respective case C models (rather than being equal or in the middle between C and F). We have analysed these deviations statistically and can confirm that

| model | O_{23} | O_{3}N_{2} | N_{2} | S_{23} | S_{33}O_{3} | Ar_{3}O_{3} | model | O_{23} | O_{3}N_{2} | N_{2} | S_{23} | S_{33}O_{3} | Ar_{3}O_{3} |
|-------|--------|-----------|------|-------|-------------|-------------|-------|--------|-----------|------|-------|-------------|-------------|
| CSp2.0 | 8.67 | 8.78 | 8.44 | 7.92 | 8.77 | 8.83 | CSh2.0 | 8.62 | 8.77 | 8.50 | 8.09 | 8.75 | 8.82 |
| HSp2.0 | 8.69 | 8.78 | 8.43 | 8.71 | 8.76 | 8.81 | HSh2.0 | 8.65 | 8.77 | 8.50 | 8.08 | 8.75 | 8.82 |
| FSp2.0 | 8.67 | 8.73 | 8.52 | 8.17 | 8.67 | 8.78 | FSh2.0 | 8.63 | 8.76 | 8.52 | 8.16 | 8.72 | 8.81 |
| CSp1.0 | 8.74 | 8.27 | 8.17 | 7.75 | 8.04 | 8.48 | CSh1.0 | 8.66 | 8.30 | 8.24 | 7.94 | 8.16 | 8.55 |
| HSp1.0 | 8.75 | 8.27 | 8.16 | 7.73 | 8.02 | 8.46 | HSh1.0 | 8.67 | 8.30 | 8.23 | 7.92 | 8.14 | 8.54 |
| FSp1.0 | 8.49 | 8.40 | 8.43 | 8.34 | 8.24 | 8.62 | FSh1.0 | 8.51 | 8.38 | 8.39 | 8.23 | 8.24 | 8.61 |
| CSp0.4 | 8.52 | 8.07 | 7.87 | 7.93 | 8.28 | 7.96 | CSh0.4 | 8.52 | 8.09 | 7.97 | 8.49 | 8.10 | 7.77 |
| HSp0.4 | 8.52 | 8.06 | 7.85 | 7.92 | 8.22 | 7.91 | HSh0.4 | 8.50 | 8.10 | 7.98 | 8.45 | 8.08 | 7.73 |
| FSp0.4 | 8.43 | 8.24 | 8.15 | 8.22 | 9.02 | 8.25 | FSh0.4 | 8.41 | 8.23 | 8.19 | 8.92 | 8.27 | 8.12 |
| CSp0.2 | 8.09 | 0.18 | 0.20 | 0.30 | 0.30 | 0.80 | CSh0.2 | 8.11 | 0.14 | 0.22 | 0.47 | 0.19 | 0.39 |
| HSp0.2 | 7.86 | 7.97 | 7.77 | 7.99 | 7.67 | 7.67 | HSh0.2 | 8.02 | 7.97 | 7.77 | 8.10 | 7.79 | 7.82 |
| FSp0.2 | 7.68 | 8.15 | 8.20 | 8.48 | 8.10 | 8.26 | FSh0.2 | 7.72 | 8.13 | 8.02 | 8.61 | 8.11 | 8.26 |
| CSp0.05 | 7.48 | 7.92 | 7.51 | 7.29 | 7.39 | 6.30 | CSh0.05 | 7.44 | 7.93 | 7.51 | 7.38 | 7.58 | 6.67 |
| HSp0.05 | 7.44 | 7.95 | 7.56 | 7.37 | 7.49 | 6.51 | HSh0.05 | 7.44 | 7.94 | 7.53 | 7.38 | 7.57 | 6.63 |
| FSp0.05 | 7.15 | 8.12 | 7.77 | 7.73 | 7.91 | 7.48 | FSh0.05 | 7.21 | 8.09 | 7.74 | 7.69 | 7.93 | 7.49 |
| \Delta | 0.33 | 0.20 | 0.26 | 0.44 | 0.52 | 0.18 | \Delta | 0.23 | 0.16 | 0.23 | 0.31 | 0.36 | 0.86 |

\(<\Delta> = 0.18, 0.15, 0.24, 0.47, 0.41, 0.47, <\Delta> = 0.12, 0.11, 0.18, 0.32, 0.23, 0.45<|\Delta|>

Table 4. Oxygen abundances derived applying various metallicity indicators to the integrated emission line spectra calculated for our models (See text for calibrations used). All abundances are given in logarithmic scale, 12 + log(O/H). The input values of 12 + log(O/H) (i.e. `the right answer`) are 8.99 (Z/Z⊙ = 2), 8.69 (Z/Z⊙ = 1), 8.29 (Z/Z⊙ = 0.4), 7.99 (Z/Z⊙ = 0.2) and 7.39 (Z/Z⊙ = 0.05). | \Delta |, the largest difference between the abundance derived from C, H and F cases are given for each model trio. The value averaged over all models, <|\Delta|>, is given in the last row of the table.
the small differences are simply due to the variance of our Monte Carlo models and do not bear any physical significance.

The reason for the systematic effect we see in the empirical abundance determinations can be understood by re-examining Figure 1 where the ionisation sequence of our model is parametrised in terms of oxygen and sulphur emission lines. The C (small symbols), H (medium symbols) and F (large symbols) form a sequence, with the case F models generally showing a lower ionisation parameter than case C and H models. The differences in the abundances derived from case C to F with the various indicators clearly reflect the different dependence of each indicator on the ionisation parameter. This can be simply shown for an idealised system. The ionisation parameter of a pure-hydrogen spherical volume of gas with number density \( N_H \) ionised by a source emitting \( Q_H \) hydrogen-ionising photons per second is defined as \( U = Q_H / (4\pi N_H R_e^2) \), where \( R_e \) is the Strömgren radius. In such a system, from the ionisation balance equation (e.g. Osterbrock, 1989, eqn 2.19) \( R_e \) is directly proportional to \( Q_H^{1/3} \) and to \( N_H^{-2/3} \), neglecting the temperature dependence of the hydrogen recombination coefficient.

For simplicity we compare the ionisation parameter of the system above, \( U_C \), ionised by only one source, to that of a similar system (F) ionised by \( N_s \) identical sources each emitting \( Q_H/N_s \) hydrogen-ionising photons per second. With these assumptions it is easy to show that the ionisation parameter, \( U_F \), for system F, measured at the Strömgren radius of each individual source is simply related to \( U_C \) by

\[
U_F = U_C \cdot N_s^{-1/2}
\]

and therefore always smaller than \( U_C \) for \( N_s > 1 \).

The magnitude of the errors in the metallicity derived by the strong line methods are significant. It is, however, true that the effects reported here represent a worst case scenario, and our extreme assumptions on stellar populations create a large dispersion in the resulting ionisation parameters, which in some cases exceeds the observed range, as seen in Figures 2 and 3. Aside from the magnitude of the \( \Delta \) values, however, a worrying aspect is the fact that the discrepancies between cases C, H and F are systematic. This can have an impact on galactic metallicity gradients determined via strong line methods, if these are calibrated via photoionisation models. In fact, if compact clusters (close to case C) and loose associations (close to case F) are randomly distributed within a given galaxy, then the systematic errors would only cause a larger scatter in the observed metallicities, but, given sufficient number statistics, they would not affect the measured metallicity gradient. However if the ratios of compact clusters to loose associations is somewhat dependent on the galactocentric distance, then the systematic errors due to stellar geometrical distributions may indeed introduce a bias on the measured galactic metallicity gradient, if the abundances are obtained from strong line methods calibrated on ab-initio models which do not reproduce the observed excitation of H \( \Pi \) regions. For example, recent work by Rosolowsky et al. (2007), presenting high resolution molecular gas maps of M33, showed a truncation in the mass distribution of giant molecular clouds (GMCs) at a galactocentric distance of 4 kpc. A recent study on the demographics of young star-forming clusters in M33 by Bastian et al. (2007) also shows the same cut-off at 4 kpc for the clusters detected. We could interpret this as tentative evidence of different star formation environments from the centre to the edge of M33, however, we prefer to postpone this discussion until more compelling observational evidence becomes available.

4 CONCLUSIONS

Following our theoretical investigation on the effects of the spatial configuration of ionisation sources on the temperature structure of H \( \Pi \) regions, we summarise our conclusions as follows:

(i) For intermediate to high metallicities (\( 0.4 \leq Z/Z_\odot \leq 2 \)), for a given gas density distribution, abundance and ionising spectral shape and intensity, a model with a central concentration of stars (case C) will result in higher ionic temperatures for high ionisation species (O\(^{2+}\), S\(^{2+}\), etc.), compared to the same model with stars fully distributed within the volume (case F). The opposite is true for ‘low’ ionisation species (e.g. O\(^+\), N\(^+\)). This results in a shallower gradients in the electron temperature distribution across the ionic species zones.

(ii) Low metallicity models (\( Z/Z_\odot \leq 0.2 \)) do not show the temperature inversion from low to high ionic species zones, rather a shift in the temperature is experienced by all ionic species zones, resulting in case F models being cooler than case C and H models.

(iii) At intermediate to high metallicity (\( Z/Z_\odot \geq 0.4 \)), models with stars distributed within the full volume are more isothermal (show lower \( t^2 \) values) than the same models with a central concentration of stars. These temperature “fluctuations” obtained for case C models are a simple consequence of a large temperature gradient. Multiple ionising sources of different temperatures at central or non-central locations do not produce significant temperature fluctuations in the ionised gas of models with \( Z/Z_\odot \geq 0.4 \).

(iv) At low metallicities (\( Z/Z_\odot \leq 0.2 \)), models with stars distributed within the full volume (case F) show larger \( t^2 \) values than the same models with a central concentration of stars. Here we are seeing the effects of true temperature “fluctuations” for case F models. The magnitude of \( t^2 (O^{2+}) \) remains however too small to have any significant effect on derived abundances.

(v) Multiple ionising sources of different temperatures at central or non-central locations are not the cause of significant temperature fluctuations in the ionised gas of our models with \( 0.05 \leq Z/Z_\odot \leq 2 \).

(vi) The relation \( t^2 (O^{+}) = t^2 (O^{2+}) \), often used in empirical studies, is NOT verified by our models. Extreme care should be taken to account for the uncertainties introduced by the use of this relation in studies seeking to apply corrections to CEL-derived abundances making use of an empirical estimation of temperature fluctuations. For our \( Z/Z_\odot = 2 \) models, \( t^2 (O^{2+}) \) is always a factor of 2 or more higher than \( t^2 (O^{+}) \), while for lower metallicities \( t^2 (O^{2+}) \) becomes lower than \( t^2 (O^{+}) \) sometimes by large factors (up to approximately 10).

(vii) For intermediate to high metallicity models, electron temperatures in the \( O^{2+} \) and \( O^{+} \) ionisation zones are shifted in opposite directions, contributing to the scatter observed in the \( T_e (O^{2+}) \) versus \( T_e (O^{+}) \) relation. We confirm that H \( \Pi \) region abundances derived on the basis of the \( T_e (O \Pi) \) alone should, therefore, be considered highly uncertain.

(viii) Metallicity indicators calibrated by grids of spherically symmetric photoionisation models may suffer a systematic bias, due to their dependence on the ionisation parameter of the system. For the same input parameters case F models will always result in smaller ionisation parameters than case C and H models. The errors estimated in this work (typically 0.3 dex, but larger in some cases) are likely to represent the worst-case scenario, but nevertheless their magnitude and their systematic nature does not allow them to be ignored.
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